p-Diacetylbenzene diethyl ketal

Inchi: InChI=1S/C18H30O4/c1-7-19-17(5,20-8-2)15-11-13-16(14-12-15)18(6,21-9-3)22-10-4/h1
InchiKey: OKYWFWIKJZITQH-UHFFFAOYSA-N
Formula: C18H30O4
SMILES: CCOC(C)(OCC)c1ccc(C(C)(OCC)OCC)cc1
Mol. weight [g/mol]: 310.43
CAS: 47189-08-2

Physical Properties

Property code	Value	Unit	Source
chs	-10465.00 ± 5.00	kJ/mol	NIST Webbook
gf	-210.86	kJ/mol	Joback Method
hf	-793.60 ± 9.00	kJ/mol	NIST Webbook
hfs	-905.80 ± 7.00	kJ/mol	NIST Webbook
hfus	25.95	kJ/mol	Joback Method
hsub	112.20	kJ/mol	NIST Webbook
hsub	112.20 ± 2.00	kJ/mol	NIST Webbook
hvap	65.65	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.178		Crippen Method
mcvol	264.200	ml/mol	McGowan Method
pc	1413.31	kPa	Joback Method
ss	493.80	J/mol×K	NIST Webbook
ss	493.80	J/mol×K	NIST Webbook
tb	726.12	K	Joback Method
tc	925.82	K	Joback Method
tf	425.32	K	Joback Method
tt	326.21 ± 0.01	K	NIST Webbook
tt	326.61 ± 0.02	K	NIST Webbook
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.11	J/mol×K	925.82	Joback Method

cpg	780.30	J/mol×K	726.12	Joback Method
cpg	863.70	J/mol×K	892.54	Joback Method
cpg	849.25	J/mol×K	859.25	Joback Method
cpg	833.70	J/mol×K	825.97	Joback Method
cpg	817.05	J/mol×K	792.69	Joback Method
cpg	799.26	J/mol×K	759.40	Joback Method
cps	460.00	J/mol×K	300.00	NIST Webbook
cps	462.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0000300	Pa×s	726.12	Joback Method
dvisc	0.0002564	Pa×s	475.45	Joback Method
dvisc	0.0005336	Pa×s	425.32	Joback Method
dvisc	0.0000405	Pa×s	675.99	Joback Method
dvisc	0.0000575	Pa×s	625.85	Joback Method
dvisc	0.0000868	Pa×s	575.72	Joback Method
dvisc	0.0001417	Pa×s	525.59	Joback Method
hfust	23.50	kJ/mol	326.20	NIST Webbook
hsubt	112.50	kJ/mol	316.50	NIST Webbook
hvapt	88.50	kJ/mol	338.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C47189082&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions

hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume