3,4-Dioxymethylenebenzylidenephenylacetonitrile

Inchi: InChI=1S/C16H11NO2/c17-10-14(13-4-2-1-3-5-13)8-12-6-7-15-16(9-12)19-11-18-15/h1-9
InchiKey: GNNCFMBWTKSMJN-RIYZIHGNSA-N
Formula: C16H11NO2
SMILES: N#CC(=Cc1ccc2c(c1)OCO2)c1ccccc1
Mol. weight [g/mol]: 249.26
CAS: 6948-55-6

Physical Properties

Property code	Value	Unit	Source
chs	-7941.00	kJ/mol	NIST Webbook
gf	390.47	kJ/mol	Joback Method
hf	178.00	kJ/mol	Joback Method
hfs	70.00	kJ/mol	NIST Webbook
hfus	37.92	kJ/mol	Joback Method
hvap	76.84	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.479		Crippen Method
mcvol	186.740	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	800.23	K	Joback Method
tc	1065.10	K	Joback Method
tf	469.23	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.16	J/mol×K	800.23	Joback Method
cpg	522.39	J/mol×K	844.37	Joback Method
cpg	533.71	J/mol×K	888.52	Joback Method
cpg	544.29	J/mol×K	932.66	Joback Method
cpg	554.31	J/mol×K	976.81	Joback Method
cpg	563.93	J/mol×K	1020.95	Joback Method
cpg	573.33	J/mol×K	1065.10	Joback Method

Sources

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=C6948556&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume