Meso-3,4-di-1-cyclohexen-1-yl-2,2,5,5-tetramethyl

Inchi: InChI=1S/C22H38/c1-21(2,3)19(17-13-9-7-10-14-17)20(22(4,5)6)18-15-11-8-12-16-18/h1
InchiKey: XIRWMTOAKDZMDH-UHFFFAOYSA-N
Formula: C22H38
SMILES: CC(C)(C)C(C1=CCCCC1)C(C1=CCCCC1)C(C)(C)C
Mol. weight [g/mol]: 302.54
CAS: 62678-54-0

Physical Properties

Property code	Value	Unit	Source
chs	-13726.30 ± 4.40	kJ/mol	NIST Webbook
gf	240.14	kJ/mol	Joback Method
hf	-244.00 ± 5.00	kJ/mol	NIST Webbook
hfs	-361.70	kJ/mol	NIST Webbook
hfus	14.06	kJ/mol	Joback Method
hsub	117.20 ± 2.40	kJ/mol	NIST Webbook
hsub	117.70	kJ/mol	NIST Webbook
hvap	64.58	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	7.312		Crippen Method
mcvol	290.520	ml/mol	McGowan Method
pc	1314.65	kPa	Joback Method
tb	752.14	K	Joback Method
tc	982.66	K	Joback Method
tf	362.34	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.86	J/mol×K	982.66	Joback Method
cpg	910.75	J/mol×K	752.14	Joback Method
cpg	936.21	J/mol×K	790.56	Joback Method
cpg	959.83	J/mol×K	828.98	Joback Method
cpg	981.76	J/mol×K	867.40	Joback Method

cpg	1002.15	J/mol×K	905.82	Joback Method
cpg	1021.13	J/mol×K	944.24	Joback Method
dvisc	0.0000345	Pa×s	752.14	Joback Method
dvisc	0.0043924	Pa×s	362.34	Joback Method
dvisc	0.0010597	Pa×s	427.31	Joback Method
dvisc	0.0003721	Pa×s	492.27	Joback Method
dvisc	0.0001668	Pa×s	557.24	Joback Method
dvisc	0.0000884	Pa×s	622.21	Joback Method
dvisc	0.0000528	Pa×s	687.17	Joback Method
hsubt	117.20 ± 2.40	kJ/mol	375.50	NIST Webbook

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=C62678540&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
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
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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