Cyclohexane, 1,1'-(2-tridecyl-1,3-propanediyl)bis-

Other names: 1-Cyclohexyl-2-(cyclohexylmethyl)pentadecane
Inchi: InChI=1S/C28H54/c1-2-3-4-5-6-7-8-9-10-11-14-23-28(24-26-19-15-12-16-20-26)25-27-21
InchiKey: YXVMXTUZMDZWJI-UHFFFAOYSA-N
Formula: C28H54
SMILES: CCCCCCCCCCCCCC(CC1CCCCC1)CC1CCCCC1
Mol. weight [g/mol]: 390.73
CAS: 55255-74-8

Physical Properties

Property code	Value	Unit	Source
gf	231.34	kJ/mol	Joback Method
hf	-517.89	kJ/mol	Joback Method
hfus	48.42	kJ/mol	Joback Method
hvap	78.39	kJ/mol	Joback Method
log10ws	-10.61		Crippen Method
logp	10.244		Crippen Method
mcvol	383.660	ml/mol	McGowan Method
pc	821.95	kPa	Joback Method
tb	878.70	K	Joback Method
tc	1081.03	K	Joback Method
tf	274.90 ± 1.00	K	NIST Webbook
tf	274.90 ± 2.00	K	NIST Webbook
vc	1.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1479.70	J/mol×K	1081.03	Joback Method
cpg	1461.87	J/mol×K	1047.31	Joback Method
cpg	1442.69	J/mol×K	1013.59	Joback Method
cpg	1422.08	J/mol×K	979.86	Joback Method
cpg	1399.97	J/mol×K	946.14	Joback Method
cpg	1376.26	J/mol×K	912.42	Joback Method
cpg	1350.90	J/mol×K	878.70	Joback Method

dvisc	0.0023623	Pa×s	405.08	Joback Method
dvisc	0.0000320	Pa×s	878.70	Joback Method
dvisc	0.0000460	Pa×s	799.76	Joback Method
dvisc	0.0000716	Pa×s	720.83	Joback Method
dvisc	0.0001243	Pa×s	641.89	Joback Method
dvisc	0.0002519	Pa×s	562.95	Joback Method
dvisc	0.0006427	Pa×s	484.02	Joback Method
hvapt	105.40	kJ/mol	518.50	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=C55255748&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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