

1,2-Cyclohexanedicarboxylic acid, 2-methoxyethyl octadecyl ester

Inchi: InChI=1S/C29H54O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-33-28(30)26-21-19-22
InchiKey: PCCYWPXTIMBIKC-UHFFFAOYSA-N
Formula: C29H54O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOC
Mol. weight [g/mol]: 482.74

Physical Properties

Property code	Value	Unit	Source
gf	-362.80	kJ/mol	Joback Method
hf	-1229.73	kJ/mol	Joback Method
hfus	70.53	kJ/mol	Joback Method
hvap	100.99	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.787		Crippen Method
mvol	429.360	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	3383.00		NIST Webbook
rinpol	3383.00		NIST Webbook
tb	1052.80	K	Joback Method
tc	1303.51	K	Joback Method
tf	586.28	K	Joback Method
vc	1.657	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1569.61	J/molxK	1052.80	Joback Method
cpg	1589.34	J/molxK	1094.58	Joback Method
cpg	1606.36	J/molxK	1136.37	Joback Method
cpg	1620.75	J/molxK	1178.15	Joback Method
cpg	1632.55	J/molxK	1219.94	Joback Method
cpg	1641.83	J/molxK	1261.72	Joback Method
cpg	1648.65	J/molxK	1303.51	Joback Method
dvisc	0.0002368	Paxs	586.28	Joback Method

dvisc	0.0001114	Paxs	664.03	Joback Method
dvisc	0.0000614	Paxs	741.79	Joback Method
dvisc	0.0000379	Paxs	819.54	Joback Method
dvisc	0.0000254	Paxs	897.29	Joback Method
dvisc	0.0000182	Paxs	975.05	Joback Method
dvisc	0.0000136	Paxs	1052.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340038&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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