

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

Inchi: InChI=1S/C30H56O5/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-34-29(31)27-22
InchiKey: ZSJQTPYPAMLGML-UHFFFAOYSA-N
Formula: C30H56O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOCC
Mol. weight [g/mol]: 496.76

Physical Properties

Property code	Value	Unit	Source
gf	-354.38	kJ/mol	Joback Method
hf	-1250.37	kJ/mol	Joback Method
hfus	73.12	kJ/mol	Joback Method
hvap	103.22	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	8.177		Crippen Method
mcvol	443.450	ml/mol	McGowan Method
pc	674.30	kPa	Joback Method
rinpol	3427.00		NIST Webbook
rinpol	3427.00		NIST Webbook
tb	1075.68	K	Joback Method
tc	1338.42	K	Joback Method
tf	597.55	K	Joback Method
vc	1.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1633.90	J/molxK	1075.68	Joback Method
cpg	1704.13	J/molxK	1294.63	Joback Method
cpg	1695.75	J/molxK	1250.84	Joback Method
cpg	1684.61	J/molxK	1207.05	Joback Method
cpg	1670.64	J/molxK	1163.26	Joback Method
cpg	1653.76	J/molxK	1119.47	Joback Method
cpg	1709.81	J/molxK	1338.42	Joback Method
dvisc	0.0000116	Paxs	1075.68	Joback Method

dvisc	0.0000155	Paxs	995.99	Joback Method
dvisc	0.0000218	Paxs	916.30	Joback Method
dvisc	0.0000325	Paxs	836.61	Joback Method
dvisc	0.0000529	Paxs	756.93	Joback Method
dvisc	0.0000966	Paxs	677.24	Joback Method
dvisc	0.0002070	Paxs	597.55	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=U339919&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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