

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

Inchi:	InChI=1S/C27H50O5/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-31-26(28)24-19-16-17-2
InchiKey:	AXXDQCMZVHYTMR-UHFFFAOYSA-N
Formula:	C27H50O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOC
Mol. weight [g/mol]:	454.68

Physical Properties

Property code	Value	Unit	Source
gf	-379.64	kJ/mol	Joback Method
hf	-1188.45	kJ/mol	Joback Method
hfus	65.35	kJ/mol	Joback Method
hvap	96.54	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	7.007		Crippen Method
mcvol	401.180	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3165.00		NIST Webbook
rinpol	3165.00		NIST Webbook
tb	1007.04	K	Joback Method
tc	1237.96	K	Joback Method
tf	563.74	K	Joback Method
vc	1.546	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.36	J/molxK	1007.04	Joback Method
cpg	1460.80	J/molxK	1045.53	Joback Method
cpg	1477.99	J/molxK	1084.01	Joback Method
cpg	1492.98	J/molxK	1122.50	Joback Method
cpg	1505.79	J/molxK	1160.99	Joback Method
cpg	1516.47	J/molxK	1199.48	Joback Method
cpg	1525.05	J/molxK	1237.96	Joback Method
dvisc	0.0003076	Paxs	563.74	Joback Method

dvisc	0.0001471	Paxs	637.62	Joback Method
dvisc	0.0000820	Paxs	711.51	Joback Method
dvisc	0.0000510	Paxs	785.39	Joback Method
dvisc	0.0000345	Paxs	859.27	Joback Method
dvisc	0.0000248	Paxs	933.16	Joback Method
dvisc	0.0000187	Paxs	1007.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340037&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

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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