

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

Inchi:	InChI=1S/C23H42O5/c1-3-4-5-6-7-8-9-10-11-14-17-27-22(24)20-15-12-13-16-21(20)23(2)
InchiKey:	ZXAGWMGWJOZOBU-UHFFFAOYSA-N
Formula:	C23H42O5
SMILES:	CCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOC
Mol. weight [g/mol]:	398.58

Physical Properties

Property code	Value	Unit	Source
gf	-413.32	kJ/mol	Joback Method
hf	-1105.89	kJ/mol	Joback Method
hfus	54.99	kJ/mol	Joback Method
hvap	87.63	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	5.447		Crippen Method
mcvol	344.820	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2743.00		NIST Webbook
tb	915.52	K	Joback Method
tc	1121.29	K	Joback Method
tf	518.66	K	Joback Method
vc	1.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.49	J/molxK	915.52	Joback Method
cpg	1265.78	J/molxK	1086.99	Joback Method
cpg	1253.39	J/molxK	1052.70	Joback Method
cpg	1239.38	J/molxK	1018.40	Joback Method
cpg	1223.74	J/molxK	984.11	Joback Method
cpg	1206.45	J/molxK	949.81	Joback Method
cpg	1276.57	J/molxK	1121.29	Joback Method
dvisc	0.0000343	Paxs	915.52	Joback Method
dvisc	0.0000451	Paxs	849.38	Joback Method

dvisc	0.0000621	Paxs	783.23	Joback Method
dvisc	0.0000906	Paxs	717.09	Joback Method
dvisc	0.0001428	Paxs	650.95	Joback Method
dvisc	0.0002496	Paxs	584.80	Joback Method
dvisc	0.0005027	Paxs	518.66	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U340034&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
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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