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

Inchi: InChI=1S/C25H46O5/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-29-24(26)22-17-14-15-18-23(2

InchiKey: KBUFKXWHGUVOAA-UHFFFAOYSA-N

Formula: C25H46O5

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCOC

Mol. weight [g/mol]: 426.63

Physical Properties

Property code	Value	Unit	Source
gf	-396.48	kJ/mol	Joback Method
hf	-1147.17	kJ/mol	Joback Method
hfus	60.17	kJ/mol	Joback Method
hvap	92.09	kJ/mol	Joback Method
log10ws	-6.51		Crippen Method
logp	6.227		Crippen Method
mcvol	373.000	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	2948.00		NIST Webbook
rinpol	2948.00		NIST Webbook
tb	961.28	K	Joback Method
tc	1177.45	K	Joback Method
tf	541.20	K	Joback Method
vc	1.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.84	J/mol×K	961.28	Joback Method
cpg	1333.02	J/mol×K	997.31	Joback Method
cpg	1350.29	J/mol×K	1033.34	Joback Method
cpg	1365.66	J/mol×K	1069.37	Joback Method
cpg	1379.18	J/mol×K	1105.40	Joback Method
cpg	1390.85	J/mol×K	1141.42	Joback Method
cpg	1400.71	J/mol×K	1177.45	Joback Method
dvisc	0.0003955	Pa×s	541.20	Joback Method

dvisc	0.0001926	Pa×s	611.21	Joback Method
dvisc	0.0001087	Pa×s	681.23	Joback Method
dvisc	0.0000683	Pa×s	751.24	Joback Method
dvisc	0.0000464	Pa×s	821.25	Joback Method
dvisc	0.0000335	Pa×s	891.27	Joback Method
dvisc	0.0000254	Pa×s	961.28	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=U340035&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