

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

Inchi:	InChI=1S/C26H48O5/c1-3-5-6-7-8-9-10-11-12-13-14-17-20-30-25(27)23-18-15-16-19-24
InchiKey:	MIQJCVLIYRYZNS-UHFFFAOYSA-N
Formula:	C26H48O5
SMILES:	CCCCCCCCCCCCCOC(=O)C1CCCC1C(=O)OCCOCC
Mol. weight [g/mol]:	440.66

Physical Properties

Property code	Value	Unit	Source
gf	-388.06	kJ/mol	Joback Method
hf	-1167.81	kJ/mol	Joback Method
hfus	62.76	kJ/mol	Joback Method
hvap	94.31	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	6.617		Crippen Method
mvol	387.090	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	2908.00		NIST Webbook
rinpol	2908.00		NIST Webbook
tb	984.16	K	Joback Method
tc	1207.12	K	Joback Method
tf	552.47	K	Joback Method
vc	1.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.48	J/molxK	984.16	Joback Method
cpg	1396.79	J/molxK	1021.32	Joback Method
cpg	1414.03	J/molxK	1058.48	Joback Method
cpg	1429.23	J/molxK	1095.64	Joback Method
cpg	1442.42	J/molxK	1132.80	Joback Method
cpg	1453.64	J/molxK	1169.96	Joback Method
cpg	1462.91	J/molxK	1207.12	Joback Method
dvisc	0.0003493	Paxs	552.47	Joback Method

dvisc	0.0001685	Paxs	624.42	Joback Method
dvisc	0.0000945	Paxs	696.37	Joback Method
dvisc	0.0000591	Paxs	768.32	Joback Method
dvisc	0.0000400	Paxs	840.26	Joback Method
dvisc	0.0000288	Paxs	912.21	Joback Method
dvisc	0.0000218	Paxs	984.16	Joback Method

Sources

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=U339915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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