1,2-Cyclohexanedicarboxylic acid, cyclohexylmethyl tetradecyl ester

Inchi: InChI=1S/C29H52O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-23-32-28(30)26-21-16-17-22-27(26

InchiKey: PIJBPYRNMVOHEZ-UHFFFAOYSA-N

Formula: C29H52O4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC1CCCCC1

Mol. weight [g/mol]: 464.72

Physical Properties

Property code	Value	Unit	Source
gf	-233.35	kJ/mol	Joback Method
hf	-1043.19	kJ/mol	Joback Method
hfus	61.18	kJ/mol	Joback Method
hvap	99.01	kJ/mol	Joback Method
log10ws	-8.75		Crippen Method
logp	8.161		Crippen Method
mcvol	412.630	ml/mol	McGowan Method
pc	801.15	kPa	Joback Method
rinpol	3337.00		NIST Webbook
rinpol	3337.00		NIST Webbook
tb	1049.93	K	Joback Method
tc	1287.06	K	Joback Method
tf	571.43	K	Joback Method
vc	1.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1534.47	J/mol×K	1049.93	Joback Method
cpg	1553.20	J/mol×K	1089.45	Joback Method
cpg	1569.57	J/mol×K	1128.97	Joback Method
cpg	1583.64	J/mol×K	1168.50	Joback Method
cpg	1595.50	J/mol×K	1208.02	Joback Method
cpg	1605.22	J/mol×K	1247.54	Joback Method
cpg	1612.87	J/mol×K	1287.06	Joback Method
dvisc	0.0003881	Pa×s	571.43	Joback Method

dvisc	0.0001727	Pa×s	651.18	Joback Method
dvisc	0.0000917	Pa×s	730.93	Joback Method
dvisc	0.0000551	Pa×s	810.68	Joback Method
dvisc	0.0000363	Pa×s	890.43	Joback Method
dvisc	0.0000256	Pa×s	970.18	Joback Method
dvisc	0.0000191	Pa×s	1049.93	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=U339747&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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