1,2-Cyclohexanedicarboxylic acid, heptyl tetradecyl ester

Inchi: InChI=1S/C29H54O4/c1-3-5-7-9-10-11-12-13-14-15-17-21-25-33-29(31)27-23-19-18-22-

InchiKey: VDFCHJRCBRRXII-UHFFFAOYSA-N

Formula: C29H54O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OCCCCCCC

Mol. weight [g/mol]: 466.74

Physical Properties

Property code	Value	Unit	Source
gf	-257.80	kJ/mol	Joback Method
hf	-1097.51	kJ/mol	Joback Method
hfus	69.35	kJ/mol	Joback Method
hvap	98.58	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.551		Crippen Method
mcvol	423.490	ml/mol	McGowan Method
pc	715.68	kPa	Joback Method
rinpol	3230.00		NIST Webbook
rinpol	3230.00		NIST Webbook
tb	1030.38	K	Joback Method
tc	1271.14	K	Joback Method
tf	564.05	K	Joback Method
vc	1.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1539.62	J/mol×K	1030.38	Joback Method
cpg	1621.57	J/mol×K	1231.01	Joback Method
cpg	1609.51	J/mol×K	1190.88	Joback Method
cpg	1595.36	J/mol×K	1150.76	Joback Method
cpg	1579.04	J/mol×K	1110.63	Joback Method
cpg	1560.49	J/mol×K	1070.51	Joback Method
cpg	1631.62	J/mol×K	1271.14	Joback Method
dvisc	0.0000186	Pa×s	1030.38	Joback Method

dvisc	0.0000249	Pa×s	952.66	Joback Method
dvisc	0.0000350	Pa×s	874.94	Joback Method
dvisc	0.0000526	Pa×s	797.22	Joback Method
dvisc	0.0000862	Pa×s	719.49	Joback Method
dvisc	0.0001595	Pa×s	641.77	Joback Method
dvisc	0.0003496	Pa×s	564.05	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=U339542&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