1,2-Cyclohexanedicarboxylic acid, heptyl pentadecyl ester

Inchi: InChI=1S/C30H56O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-22-26-34-30(32)28-24-20-19-

InchiKey: GPSCEVFREBAQSZ-UHFFFAOYSA-N

Formula: C30H56O4

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

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-249.38	kJ/mol	Joback Method
hf	-1118.15	kJ/mol	Joback Method
hfus	71.94	kJ/mol	Joback Method
hvap	100.81	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.941		Crippen Method
mcvol	437.580	ml/mol	McGowan Method
pc	680.29	kPa	Joback Method
rinpol	3345.00		NIST Webbook
rinpol	3345.00		NIST Webbook
tb	1053.26	K	Joback Method
tc	1304.73	K	Joback Method
tf	575.32	K	Joback Method
vc	1.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.51	J/mol×K	1053.26	Joback Method
cpg	1625.68	J/mol×K	1095.17	Joback Method
cpg	1644.32	J/mol×K	1137.08	Joback Method
cpg	1660.52	J/mol×K	1179.00	Joback Method
cpg	1674.38	J/mol×K	1220.91	Joback Method
cpg	1685.97	J/mol×K	1262.82	Joback Method
cpg	1695.39	J/mol×K	1304.73	Joback Method
dvisc	0.0003062	Pa×s	575.32	Joback Method

dvisc	0.0001386	Pa×s	654.98	Joback Method
dvisc	0.0000745	Pa×s	734.63	Joback Method
dvisc	0.0000452	Pa×s	814.29	Joback Method
dvisc	0.0000300	Pa×s	893.95	Joback Method
dvisc	0.0000213	Pa×s	973.60	Joback Method
dvisc	0.0000159	Pa×s	1053.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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