1,2-Cyclohexanedicarboxylic acid, hexadecyl 2-methylpent-3-yl ester

Inchi: InChI=1S/C30H56O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-29(31)26-22-19-

InchiKey: JWMIOWVEESAQGL-UHFFFAOYSA-N

Formula: C30H56O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(CC)C(C)C

Mol. weight [g/mol]: 480.76

Physical Properties

Property code	Value	Unit	Source
gf	-254.26	kJ/mol	Joback Method
hf	-1128.71	kJ/mol	Joback Method
hfus	64.89	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-9.39		Crippen Method
logp	8.795		Crippen Method
mcvol	437.580	ml/mol	McGowan Method
pc	686.01	kPa	Joback Method
rinpol	3324.00		NIST Webbook
rinpol	3324.00		NIST Webbook
tb	1052.38	K	Joback Method
tc	1299.39	K	Joback Method
tf	545.32	K	Joback Method
vc	1.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.88	J/mol×K	1052.38	Joback Method
cpg	1684.21	J/mol×K	1258.22	Joback Method
cpg	1672.96	J/mol×K	1217.06	Joback Method
cpg	1659.48	J/mol×K	1175.89	Joback Method
cpg	1643.70	J/mol×K	1134.72	Joback Method
cpg	1625.53	J/mol×K	1093.55	Joback Method
cpg	1693.33	J/mol×K	1299.39	Joback Method
dvisc	0.0000131	Pa×s	1052.38	Joback Method

dvisc	0.0000180	Pa×s	967.87	Joback Method
dvisc	0.0000263	Pa×s	883.36	Joback Method
dvisc	0.0000416	Pa×s	798.85	Joback Method
dvisc	0.0000733	Pa×s	714.34	Joback Method
dvisc	0.0001503	Pa×s	629.83	Joback Method
dvisc	0.0003850	Pa×s	545.32	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U339450&Units=SI

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