

1,2-Cyclohexanedicarboxylic acid, heptadecyl 3-methylbut-2-yl ester

Inchi:	InChI=1S/C30H56O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-24-33-29(31)27-22-1
InchiKey:	IKHWJLIAYCKPPI-UHFFFAOYSA-N
Formula:	C30H56O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC(C)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	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1052.38	K	Joback Method
tc	1299.39	K	Joback Method
tf	545.32	K	Joback Method
vc	1.683	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1604.88	J/molxK	1052.38	Joback Method
cpg	1625.53	J/molxK	1093.55	Joback Method
cpg	1643.70	J/molxK	1134.72	Joback Method
cpg	1659.48	J/molxK	1175.89	Joback Method
cpg	1672.96	J/molxK	1217.06	Joback Method
cpg	1684.21	J/molxK	1258.22	Joback Method
cpg	1693.33	J/molxK	1299.39	Joback Method
dvisc	0.0003850	Paxs	545.32	Joback Method

dvisc	0.0001503	Paxs	629.83	Joback Method
dvisc	0.0000733	Paxs	714.34	Joback Method
dvisc	0.0000416	Paxs	798.85	Joback Method
dvisc	0.0000263	Paxs	883.36	Joback Method
dvisc	0.0000180	Paxs	967.87	Joback Method
dvisc	0.0000131	Paxs	1052.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U339569&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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