

1,2-Cyclohexanedicarboxylic acid, hexadecyl methyl ester

Inchi:	InChI=1S/C25H46O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-29-25(27)23-20-17-16-
InchiKey:	INIZGHVNWBSUAS-UHFFFAOYSA-N
Formula:	C25H46O4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)C1CCCCC1C(=O)OC
Mol. weight [g/mol]:	410.63

Physical Properties

Property code	Value	Unit	Source
gf	-291.48	kJ/mol	Joback Method
hf	-1014.95	kJ/mol	Joback Method
hfus	58.99	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	6.990		Crippen Method
mvol	367.130	ml/mol	McGowan Method
pc	888.94	kPa	Joback Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook
tb	938.86	K	Joback Method
tc	1149.44	K	Joback Method
tf	518.97	K	Joback Method
vc	1.415	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1282.28	J/molxK	938.86	Joback Method
cpg	1302.20	J/molxK	973.96	Joback Method
cpg	1320.41	J/molxK	1009.05	Joback Method
cpg	1336.95	J/molxK	1044.15	Joback Method
cpg	1351.86	J/molxK	1079.25	Joback Method
cpg	1365.17	J/molxK	1114.35	Joback Method
cpg	1376.92	J/molxK	1149.44	Joback Method
dvisc	0.0005793	Paxs	518.97	Joback Method

dvisc	0.0002735	Paxs	588.95	Joback Method
dvisc	0.0001515	Paxs	658.93	Joback Method
dvisc	0.0000939	Paxs	728.91	Joback Method
dvisc	0.0000634	Paxs	798.90	Joback Method
dvisc	0.0000455	Paxs	868.88	Joback Method
dvisc	0.0000344	Paxs	938.86	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=U339662&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

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