

1,2-Cyclohexanedicarboxylic acid, isobutyl undecyl ester

Inchi:	InChI=1S/C23H42O4/c1-4-5-6-7-8-9-10-11-14-17-26-22(24)20-15-12-13-16-21(20)23(25)
InchiKey:	KFFISQLLHSGQKG-UHFFFAOYSA-N
Formula:	C23H42O4
SMILES:	CCCCCCCCCOC(=O)C1CCCCC1C(=O)OCC(C)C
Mol. weight [g/mol]:	382.58

Physical Properties

Property code	Value	Unit	Source
gf	-310.76	kJ/mol	Joback Method
hf	-978.95	kJ/mol	Joback Method
hfus	50.28	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	6.066		Crippen Method
mvol	338.950	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	2596.00		NIST Webbook
rinpol	2596.00		NIST Webbook
tb	892.66	K	Joback Method
tc	1095.22	K	Joback Method
tf	481.43	K	Joback Method
vc	1.298	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.06	J/molxK	892.66	Joback Method
cpg	1175.71	J/molxK	926.42	Joback Method
cpg	1193.82	J/molxK	960.18	Joback Method
cpg	1210.41	J/molxK	993.94	Joback Method
cpg	1225.52	J/molxK	1027.70	Joback Method
cpg	1239.17	J/molxK	1061.46	Joback Method
cpg	1251.39	J/molxK	1095.22	Joback Method
dvisc	0.0008412	Paxs	481.43	Joback Method

dvisc	0.0003744	Paxs	549.97	Joback Method
dvisc	0.0001994	Paxs	618.51	Joback Method
dvisc	0.0001204	Paxs	687.04	Joback Method
dvisc	0.0000797	Paxs	755.58	Joback Method
dvisc	0.0000565	Paxs	824.12	Joback Method
dvisc	0.0000422	Paxs	892.66	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=U339432&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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