

1,2-Cyclohexanedicarboxylic acid, cyclohex-3-enylmethyl isobutyl ester

Inchi: InChI=1S/C19H30O4/c1-14(2)12-22-18(20)16-10-6-7-11-17(16)19(21)23-13-15-8-4-3-5-9
InchiKey: YUCZHEXLLRNOJX-UHFFFAOYSA-N
Formula: C19H30O4
SMILES: CC(C)COC(=O)C1CCCCC1C(=O)OCC1CC=CCC1
Mol. weight [g/mol]: 322.44

Physical Properties

Property code	Value	Unit	Source
gf	-290.03	kJ/mol	Joback Method
hf	-784.29	kJ/mol	Joback Method
hfus	32.98	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.891		Crippen Method
mcvol	267.430	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2270.00		NIST Webbook
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tb	819.85	K	Joback Method
tc	1039.43	K	Joback Method
tf	444.49	K	Joback Method
vc	0.993	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.51	J/molxK	819.85	Joback Method
cpg	898.50	J/molxK	856.45	Joback Method
cpg	916.78	J/molxK	893.04	Joback Method
cpg	933.37	J/molxK	929.64	Joback Method
cpg	948.31	J/molxK	966.24	Joback Method
cpg	961.61	J/molxK	1002.83	Joback Method
cpg	973.31	J/molxK	1039.43	Joback Method
dvisc	0.0014560	Paxs	444.49	Joback Method

dvisc	0.0006732	Paxs	507.05	Joback Method
dvisc	0.0003688	Paxs	569.61	Joback Method
dvisc	0.0002275	Paxs	632.17	Joback Method
dvisc	0.0001532	Paxs	694.73	Joback Method
dvisc	0.0001101	Paxs	757.29	Joback Method
dvisc	0.0000832	Paxs	819.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U339867&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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