

1,2-Cyclohexanedicarboxylic acid, isohexyl pentyl ester

Inchi:	InChI=1S/C19H34O4/c1-4-5-8-13-22-18(20)16-11-6-7-12-17(16)19(21)23-14-9-10-15(2)3
InchiKey:	VBWRYUFWLNSTMW-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCCOC(=O)C1CCCCC1C(=O)OCCCC(C)C
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-344.44	kJ/mol	Joback Method
hf	-896.39	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.506		Crippen Method
mcvol	282.590	ml/mol	McGowan Method
pc	1303.29	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	801.14	K	Joback Method
tc	997.68	K	Joback Method
tf	436.35	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.24	J/molxK	801.14	Joback Method
cpg	928.59	J/molxK	833.90	Joback Method
cpg	946.62	J/molxK	866.65	Joback Method
cpg	963.37	J/molxK	899.41	Joback Method
cpg	978.84	J/molxK	932.17	Joback Method
cpg	993.04	J/molxK	964.93	Joback Method
cpg	1006.00	J/molxK	997.68	Joback Method
dvisc	0.0013131	Paxs	436.35	Joback Method

dvisc	0.0006075	Paxs	497.15	Joback Method
dvisc	0.0003324	Paxs	557.95	Joback Method
dvisc	0.0002048	Paxs	618.75	Joback Method
dvisc	0.0001376	Paxs	679.54	Joback Method
dvisc	0.0000987	Paxs	740.34	Joback Method
dvisc	0.0000744	Paxs	801.14	Joback Method

Sources

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=U339468&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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