

Diisobutyl 2-cyclohexene-1,4-dicarboxylate

Inchi:	InChI=1S/C16H26O4/c1-11(2)9-19-15(17)13-5-7-14(8-6-13)16(18)20-10-12(3)4/h5,7,11-
InchiKey:	ZORBITPFPDERNE-UHFFFAOYSA-N
Formula:	C16H26O4
SMILES:	CC(C)COC(=O)C1C=CC(C(=O)OCC(C)C)CC1
Mol. weight [g/mol]:	282.38

Physical Properties

Property code	Value	Unit	Source
gf	-342.18	kJ/mol	Joback Method
hf	-781.97	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.967		Crippen Method
mcvol	236.020	ml/mol	McGowan Method
pc	1682.41	kPa	Joback Method
tb	731.22	K	Joback Method
tc	934.41	K	Joback Method
tf	388.30	K	Joback Method
vc	0.885	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.16	J/molxK	731.22	Joback Method
cpg	787.70	J/molxK	900.55	Joback Method
cpg	773.96	J/molxK	866.68	Joback Method
cpg	759.05	J/molxK	832.82	Joback Method
cpg	742.95	J/molxK	798.95	Joback Method
cpg	725.65	J/molxK	765.09	Joback Method
cpg	800.27	J/molxK	934.41	Joback Method
dvisc	0.0001081	Paxs	731.22	Joback Method
dvisc	0.0001429	Paxs	674.07	Joback Method
dvisc	0.0001990	Paxs	616.91	Joback Method

dvisc	0.0002966	Paxs	559.76	Joback Method
dvisc	0.0004839	Paxs	502.61	Joback Method
dvisc	0.0008952	Paxs	445.45	Joback Method
dvisc	0.0019850	Paxs	388.30	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=B6009660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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