

Dimethylmalonic acid, isobutyl trans-4-methylcyclohexyl ester

Inchi:	InChI=1S/C16H28O4/c1-11(2)10-19-14(17)16(4,5)15(18)20-13-8-6-12(3)7-9-13/h11-13H
InchiKey:	DUAMWUBVOSLGCE-UHFFFAOYSA-N
Formula:	C16H28O4
SMILES:	CC(C)COC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	284.39

Physical Properties

Property code	Value	Unit	Source
gf	-366.86	kJ/mol	Joback Method
hf	-843.22	kJ/mol	Joback Method
hfus	24.74	kJ/mol	Joback Method
hvap	67.96	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.334		Crippen Method
mcvol	240.320	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1760.00		NIST Webbook
tb	729.27	K	Joback Method
tc	936.90	K	Joback Method
tf	404.96	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.80	J/molxK	729.27	Joback Method
cpg	753.42	J/molxK	763.87	Joback Method
cpg	771.73	J/molxK	798.48	Joback Method
cpg	788.74	J/molxK	833.08	Joback Method
cpg	804.50	J/molxK	867.69	Joback Method
cpg	819.02	J/molxK	902.29	Joback Method
cpg	832.32	J/molxK	936.90	Joback Method
dvisc	0.0017904	Paxs	404.96	Joback Method
dvisc	0.0008145	Paxs	459.01	Joback Method

dvisc	0.0004374	Paxs	513.06	Joback Method
dvisc	0.0002645	Paxs	567.12	Joback Method
dvisc	0.0001746	Paxs	621.17	Joback Method
dvisc	0.0001231	Paxs	675.22	Joback Method
dvisc	0.0000915	Paxs	729.27	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=U363895&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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