

Dimethylmalonic acid, cis-4-methylcyclohexyl propyl ester

Inchi:	InChI=1S/C15H26O4/c1-5-10-18-13(16)15(3,4)14(17)19-12-8-6-11(2)7-9-12/h11-12H,5-
InchiKey:	LTWDJISZAVEHMD-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	CCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-372.84	kJ/mol	Joback Method
hf	-817.30	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	66.12	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	3.088		Crippen Method
mcvol	226.230	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinsol	1758.00		NIST Webbook
tb	706.83	K	Joback Method
tc	913.56	K	Joback Method
tf	408.69	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.37	J/molxK	706.83	Joback Method
cpg	760.07	J/molxK	879.11	Joback Method
cpg	745.72	J/molxK	844.65	Joback Method
cpg	730.20	J/molxK	810.20	Joback Method
cpg	713.49	J/molxK	775.74	Joback Method
cpg	695.55	J/molxK	741.29	Joback Method
cpg	773.26	J/molxK	913.56	Joback Method
dvisc	0.0001132	Paxs	706.83	Joback Method
dvisc	0.0001492	Paxs	657.14	Joback Method

dvisc	0.0002056	Paxs	607.45	Joback Method
dvisc	0.0003000	Paxs	557.76	Joback Method
dvisc	0.0004713	Paxs	508.07	Joback Method
dvisc	0.0008167	Paxs	458.38	Joback Method
dvisc	0.0016175	Paxs	408.69	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=U363875&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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