

Dimethylmalonic acid, cis-4-methylcyclohexyl ethyl ester

Inchi:	InChI=1S/C14H24O4/c1-5-17-12(15)14(3,4)13(16)18-11-8-6-10(2)7-9-11/h10-11H,5-9H2
InchiKey:	HRVOFSXIGCWMSS-UHFFFAOYSA-N
Formula:	C14H24O4
SMILES:	CCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	256.34

Physical Properties

Property code	Value	Unit	Source
gf	-381.26	kJ/mol	Joback Method
hf	-796.66	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	63.89	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.698		Crippen Method
mvol	212.140	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	683.95	K	Joback Method
tc	893.46	K	Joback Method
tf	397.42	K	Joback Method
vc	0.788	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.51	J/molxK	683.95	Joback Method
cpg	639.53	J/molxK	718.87	Joback Method
cpg	657.32	J/molxK	753.79	Joback Method
cpg	673.90	J/molxK	788.71	Joback Method
cpg	689.31	J/molxK	823.63	Joback Method
cpg	703.56	J/molxK	858.54	Joback Method
cpg	716.67	J/molxK	893.46	Joback Method
dvisc	0.0017655	Paxs	397.42	Joback Method

dvisc	0.0009034	Paxs	445.18	Joback Method
dvisc	0.0005263	Paxs	492.93	Joback Method
dvisc	0.0003374	Paxs	540.68	Joback Method
dvisc	0.0002324	Paxs	588.44	Joback Method
dvisc	0.0001693	Paxs	636.19	Joback Method
dvisc	0.0001290	Paxs	683.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363874&Units=SI
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

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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