

Dimethylmalonic acid, heptyl trans-4-methylcyclohexyl ester

Inchi:	InChI=1S/C19H34O4/c1-5-6-7-8-9-14-22-17(20)19(3,4)18(21)23-16-12-10-15(2)11-13-16
InchiKey:	FIJNKZQKLJVVSE-UHFFFAOYSA-N
Formula:	C19H34O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)OC1CCC(C)CC1
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-339.16	kJ/mol	Joback Method
hf	-899.86	kJ/mol	Joback Method
hfus	36.03	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.648		Crippen Method
mvol	282.590	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2099.00		NIST Webbook
rinpol	2099.00		NIST Webbook
tb	798.35	K	Joback Method
tc	998.71	K	Joback Method
tf	453.77	K	Joback Method
vc	1.069	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.86	J/molxK	798.35	Joback Method
cpg	929.33	J/molxK	831.74	Joback Method
cpg	947.46	J/molxK	865.14	Joback Method
cpg	964.30	J/molxK	898.53	Joback Method
cpg	979.86	J/molxK	931.92	Joback Method
cpg	994.19	J/molxK	965.32	Joback Method
cpg	1007.31	J/molxK	998.71	Joback Method
dvisc	0.0010802	Paxs	453.77	Joback Method

dvisc	0.0005200	Paxs	511.20	Joback Method
dvisc	0.0002901	Paxs	568.63	Joback Method
dvisc	0.0001802	Paxs	626.06	Joback Method
dvisc	0.0001212	Paxs	683.49	Joback Method
dvisc	0.0000867	Paxs	740.92	Joback Method
dvisc	0.0000651	Paxs	798.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363899&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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