Dimethylmalonic acid, cis-4-methylcyclohexyl heptyl 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: FIJNKZQKLJVWSE-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
mcvol	282.590	ml/mol	McGowan Method
pc	1313.70	kPa	Joback Method
rinpol	2138.00		NIST Webbook
rinpol	2138.00		NIST Webbook
tb	798.35	K	Joback Method
tc	998.71	K	Joback Method
tf	453.77	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0005200	Pa×s	511.20	Joback Method
dvisc	0.0002901	Pa×s	568.63	Joback Method
dvisc	0.0001802	Pa×s	626.06	Joback Method
dvisc	0.0001212	Pa×s	683.49	Joback Method
dvisc	0.0000867	Pa×s	740.92	Joback Method
dvisc	0.0000651	Pa×s	798.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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