Dimethylmalonic acid, neopentyl octyl ester

Inchi: InChI=1S/C18H34O4/c1-7-8-9-10-11-12-13-21-15(19)18(5,6)16(20)22-14-17(2,3)4/h7-14
InchiKey: XCGBELQNCMMJGF-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-361.48	kJ/mol	Joback Method
hf	-921.95	kJ/mol	Joback Method
hfus	33.12	kJ/mol	Joback Method
hvap	71.38	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.506		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	1838.00		NIST Webbook
rinpol	1838.00		NIST Webbook
tb	757.36	K	Joback Method
tc	944.92	K	Joback Method
tf	441.78	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.64	J/mol×K	757.36	Joback Method
cpg	870.42	J/mol×K	788.62	Joback Method
cpg	887.18	J/mol×K	819.88	Joback Method
cpg	902.97	J/mol×K	851.14	Joback Method
cpg	917.81	J/mol×K	882.40	Joback Method
cpg	931.76	J/mol×K	913.66	Joback Method
cpg	944.84	J/mol×K	944.92	Joback Method
dvisc	0.0009881	Pa×s	441.78	Joback Method

dvisc	0.0004547	Pa×s	494.38	Joback Method
dvisc	0.0002429	Pa×s	546.97	Joback Method
dvisc	0.0001449	Pa×s	599.57	Joback Method
dvisc	0.0000939	Pa×s	652.17	Joback Method
dvisc	0.0000649	Pa×s	704.76	Joback Method
dvisc	0.0000473	Pa×s	757.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361749&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

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