

Dimethylmalonic acid, heptyl neopentyl ester

Inchi:	InChI=1S/C17H32O4/c1-7-8-9-10-11-12-20-14(18)17(5,6)15(19)21-13-16(2,3)4/h7-13H2
InchiKey:	SSJXMOZVGABOSE-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-369.90	kJ/mol	Joback Method
hf	-901.31	kJ/mol	Joback Method
hfus	30.53	kJ/mol	Joback Method
hvap	69.16	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	4.115		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	1741.00		NIST Webbook
rinpol	1741.00		NIST Webbook
tb	734.48	K	Joback Method
tc	922.17	K	Joback Method
tf	430.51	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.73	J/molxK	734.48	Joback Method
cpg	812.24	J/molxK	765.76	Joback Method
cpg	828.76	J/molxK	797.04	Joback Method
cpg	844.32	J/molxK	828.32	Joback Method
cpg	858.96	J/molxK	859.60	Joback Method
cpg	872.72	J/molxK	890.89	Joback Method
cpg	885.63	J/molxK	922.17	Joback Method
dvisc	0.0011204	Paxs	430.51	Joback Method

dvisc	0.0005212	Paxs	481.17	Joback Method
dvisc	0.0002806	Paxs	531.83	Joback Method
dvisc	0.0001682	Paxs	582.50	Joback Method
dvisc	0.0001094	Paxs	633.16	Joback Method
dvisc	0.0000759	Paxs	683.82	Joback Method
dvisc	0.0000553	Paxs	734.48	Joback Method

Sources

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=U361748&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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