

Dimethylmalonic acid, butyl octyl ester

Inchi:	InChI=1S/C17H32O4/c1-5-7-9-10-11-12-14-21-16(19)17(3,4)15(18)20-13-8-6-2/h5-14H2
InchiKey:	KZXAQCDYRDCKCI-UHFFFAOYSA-N
Formula:	C17H32O4
SMILES:	CCCCCCCCOC(=O)C(C)(C)C(=O)OCCCC
Mol. weight [g/mol]:	300.43

Physical Properties

Property code	Value	Unit	Source
gf	-372.74	kJ/mol	Joback Method
hf	-892.56	kJ/mol	Joback Method
hfus	37.95	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	4.260		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	1840.00		NIST Webbook
tb	737.71	K	Joback Method
tc	919.59	K	Joback Method
tf	428.09	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.85	J/molxK	737.71	Joback Method
cpg	810.06	J/molxK	768.02	Joback Method
cpg	826.34	J/molxK	798.34	Joback Method
cpg	841.73	J/molxK	828.65	Joback Method
cpg	856.24	J/molxK	858.97	Joback Method
cpg	869.90	J/molxK	889.28	Joback Method
cpg	882.72	J/molxK	919.59	Joback Method
dvisc	0.0011352	Paxs	428.09	Joback Method
dvisc	0.0005494	Paxs	479.69	Joback Method

dvisc	0.0003061	Paxs	531.30	Joback Method
dvisc	0.0001892	Paxs	582.90	Joback Method
dvisc	0.0001264	Paxs	634.50	Joback Method
dvisc	0.0000898	Paxs	686.11	Joback Method
dvisc	0.0000669	Paxs	737.71	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361670&Units=SI

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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