

Dimethylmalonic acid, di(4-octyl) ester

Inchi:	InChI=1S/C21H40O4/c1-7-11-15-17(13-9-3)24-19(22)21(5,6)20(23)25-18(14-10-4)16-12
InchiKey:	RVDWBJQVZXIIMG-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCC(CCC)OC(=O)C(C)(C)C(=O)OC(CCC)CCCC
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-343.94	kJ/mol	Joback Method
hf	-985.68	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.817		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	1959.00		NIST Webbook
tb	828.35	K	Joback Method
tc	1018.59	K	Joback Method
tf	443.17	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.95	J/molxK	828.35	Joback Method
cpg	1050.71	J/molxK	860.06	Joback Method
cpg	1068.32	J/molxK	891.76	Joback Method
cpg	1084.83	J/molxK	923.47	Joback Method
cpg	1100.26	J/molxK	955.18	Joback Method
cpg	1114.66	J/molxK	986.89	Joback Method
cpg	1128.05	J/molxK	1018.59	Joback Method
dvisc	0.0010254	Paxs	443.17	Joback Method
dvisc	0.0003951	Paxs	507.37	Joback Method

dvisc	0.0001886	Paxs	571.56	Joback Method
dvisc	0.0001045	Paxs	635.76	Joback Method
dvisc	0.0000646	Paxs	699.96	Joback Method
dvisc	0.0000432	Paxs	764.15	Joback Method
dvisc	0.0000308	Paxs	828.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361741&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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