

Dimethylmalonic acid, pentyl undecyl ester

Inchi:	InChI=1S/C21H40O4/c1-5-7-9-10-11-12-13-14-16-18-25-20(23)21(3,4)19(22)24-17-15-8
InchiKey:	HYQSENOLWWWQHG-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCC
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-339.06	kJ/mol	Joback Method
hf	-975.12	kJ/mol	Joback Method
hfus	48.31	kJ/mol	Joback Method
hvap	79.36	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.820		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1025.31	kPa	Joback Method
rinpol	2221.00		NIST Webbook
tb	829.23	K	Joback Method
tc	1017.76	K	Joback Method
tf	473.17	K	Joback Method
vc	1.248	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.00	J/molxK	829.23	Joback Method
cpg	1049.60	J/molxK	860.65	Joback Method
cpg	1067.09	J/molxK	892.07	Joback Method
cpg	1083.51	J/molxK	923.49	Joback Method
cpg	1098.90	J/molxK	954.91	Joback Method
cpg	1113.29	J/molxK	986.33	Joback Method
cpg	1126.71	J/molxK	1017.76	Joback Method
dvisc	0.0007084	Paxs	473.17	Joback Method
dvisc	0.0003284	Paxs	532.51	Joback Method

dvisc	0.0001776	Paxs	591.86	Joback Method
dvisc	0.0001074	Paxs	651.20	Joback Method
dvisc	0.0000707	Paxs	710.54	Joback Method
dvisc	0.0000496	Paxs	769.89	Joback Method
dvisc	0.0000366	Paxs	829.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361779&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

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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