

Dimethylmalonic acid, neopentyl undecyl ester

Inchi:	InChI=1S/C21H40O4/c1-7-8-9-10-11-12-13-14-15-16-24-18(22)21(5,6)19(23)25-17-20(2
InchiKey:	VGPSEUWAQTUJLR-UHFFFAOYSA-N
Formula:	C21H40O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	356.54

Physical Properties

Property code	Value	Unit	Source
gf	-336.22	kJ/mol	Joback Method
hf	-983.87	kJ/mol	Joback Method
hfus	40.89	kJ/mol	Joback Method
hvap	78.06	kJ/mol	Joback Method
log10ws	-5.85		Crippen Method
logp	5.676		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1037.90	kPa	Joback Method
rinpol	2133.00		NIST Webbook
tb	826.00	K	Joback Method
tc	1016.84	K	Joback Method
tf	475.59	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.80	J/molxK	826.00	Joback Method
cpg	1050.40	J/molxK	857.81	Joback Method
cpg	1067.89	J/molxK	889.61	Joback Method
cpg	1084.33	J/molxK	921.42	Joback Method
cpg	1099.76	J/molxK	953.23	Joback Method
cpg	1114.22	J/molxK	985.04	Joback Method
cpg	1127.78	J/molxK	1016.84	Joback Method
dvisc	0.0006649	Paxs	475.59	Joback Method
dvisc	0.0002970	Paxs	533.99	Joback Method

dvisc	0.0001555	Paxs	592.39	Joback Method
dvisc	0.0000914	Paxs	650.80	Joback Method
dvisc	0.0000587	Paxs	709.20	Joback Method
dvisc	0.0000403	Paxs	767.60	Joback Method
dvisc	0.0000292	Paxs	826.00	Joback Method

Sources

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=U361751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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