

Dimethylmalonic acid, decyl neopentyl ester

Inchi:	InChI=1S/C20H38O4/c1-7-8-9-10-11-12-13-14-15-23-17(21)20(5,6)18(22)24-16-19(2,3)4
InchiKey:	LXAURAQOXFMZBS-UHFFFAOYSA-N
Formula:	C20H38O4
SMILES:	CCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	342.51

Physical Properties

Property code	Value	Unit	Source
gf	-344.64	kJ/mol	Joback Method
hf	-963.23	kJ/mol	Joback Method
hfus	38.30	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.286		Crippen Method
mcvol	307.540	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinsol	2035.00		NIST Webbook
tb	803.12	K	Joback Method
tc	992.21	K	Joback Method
tf	464.32	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.25	J/mol×K	803.12	Joback Method
cpg	989.56	J/mol×K	834.63	Joback Method
cpg	1006.80	J/mol×K	866.15	Joback Method
cpg	1023.01	J/mol×K	897.66	Joback Method
cpg	1038.24	J/mol×K	929.18	Joback Method
cpg	1052.53	J/mol×K	960.69	Joback Method
cpg	1065.94	J/mol×K	992.21	Joback Method
dvisc	0.0007610	Paxs	464.32	Joback Method
dvisc	0.0003431	Paxs	520.79	Joback Method

dvisc	0.0001808	Paxs	577.25	Joback Method
dvisc	0.0001068	Paxs	633.72	Joback Method
dvisc	0.0000687	Paxs	690.19	Joback Method
dvisc	0.0000473	Paxs	746.65	Joback Method
dvisc	0.0000343	Paxs	803.12	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=U361750&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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