

Dimethylmalonic acid, neopentyl octadecyl ester

Inchi:	InChI=1S/C28H54O4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-31-25(29)28
InchiKey:	PFJSKCVYUPHQV-UHFFFAOYSA-N
Formula:	C28H54O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCC(C)(C)C
Mol. weight [g/mol]:	454.73

Physical Properties

Property code	Value	Unit	Source
gf	-277.28	kJ/mol	Joback Method
hf	-1128.35	kJ/mol	Joback Method
hfus	59.02	kJ/mol	Joback Method
hvap	93.64	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	8.407		Crippen Method
mvol	420.260	ml/mol	McGowan Method
pc	701.35	kPa	Joback Method
rinpol	2823.00		NIST Webbook
tb	986.16	K	Joback Method
tc	1213.67	K	Joback Method
tf	554.48	K	Joback Method
vc	1.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1473.71	J/molxK	986.16	Joback Method
cpg	1568.09	J/molxK	1175.75	Joback Method
cpg	1551.90	J/molxK	1137.83	Joback Method
cpg	1534.48	J/molxK	1099.92	Joback Method
cpg	1515.72	J/molxK	1062.00	Joback Method
cpg	1495.50	J/molxK	1024.08	Joback Method
cpg	1583.15	J/molxK	1213.67	Joback Method
dvisc	0.0000090	Paxs	986.16	Joback Method
dvisc	0.0000126	Paxs	914.21	Joback Method

dvisc	0.0000186	Paxs	842.27	Joback Method
dvisc	0.0000295	Paxs	770.32	Joback Method
dvisc	0.0000515	Paxs	698.37	Joback Method
dvisc	0.0001022	Paxs	626.43	Joback Method
dvisc	0.0002423	Paxs	554.48	Joback Method

Sources

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=U361758&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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