

Dimethylmalonic acid, octyl tridecyl ester

Inchi:	InChI=1S/C26H50O4/c1-5-7-9-11-13-14-15-16-17-19-21-23-30-25(28)26(3,4)24(27)29-2
InchiKey:	ITYVPRAWCXBNPY-UHFFFAOYSA-N
Formula:	C26H50O4
SMILES:	CCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OCCCCCCCC
Mol. weight [g/mol]:	426.67

Physical Properties

Property code	Value	Unit	Source
gf	-296.96	kJ/mol	Joback Method
hf	-1078.32	kJ/mol	Joback Method
hfus	61.26	kJ/mol	Joback Method
hvap	90.49	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	7.771		Crippen Method
mvol	392.080	ml/mol	McGowan Method
pc	770.32	kPa	Joback Method
rinpol	2691.00		NIST Webbook
rinpol	2691.00		NIST Webbook
tb	943.63	K	Joback Method
tc	1158.72	K	Joback Method
tf	529.52	K	Joback Method
vc	1.528	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1344.97	J/molxK	943.63	Joback Method
cpg	1435.13	J/molxK	1122.87	Joback Method
cpg	1419.86	J/molxK	1087.02	Joback Method
cpg	1403.28	J/molxK	1051.17	Joback Method
cpg	1385.32	J/molxK	1015.33	Joback Method
cpg	1365.90	J/molxK	979.48	Joback Method
cpg	1449.14	J/molxK	1158.72	Joback Method
dvisc	0.0000166	Paxs	943.63	Joback Method

dvisc	0.0000226	Paxs	874.61	Joback Method
dvisc	0.0000326	Paxs	805.59	Joback Method
dvisc	0.0000504	Paxs	736.58	Joback Method
dvisc	0.0000851	Paxs	667.56	Joback Method
dvisc	0.0001622	Paxs	598.54	Joback Method
dvisc	0.0003659	Paxs	529.52	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=U361680&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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