

Dimethylmalonic acid, hexadecyl 2-pentyl ester

Inchi: InChI=1S/C26H50O4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-22-29-24(27)26(4,5)2
InchiKey: QKRPSEGQAJXFFC-UHFFFAOYSA-N
Formula: C26H50O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(C)CCC
Mol. weight [g/mol]: 426.67

Physical Properties

Property code	Value	Unit	Source
gf	-299.40	kJ/mol	Joback Method
hf	-1083.60	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	90.10	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.769		Crippen Method
mcvol	392.080	ml/mol	McGowan Method
pc	773.75	kPa	Joback Method
rinpol	2680.00		NIST Webbook
tb	943.19	K	Joback Method
tc	1157.23	K	Joback Method
tf	514.52	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1345.34	J/mol×K	943.19	Joback Method
cpg	1366.13	J/mol×K	978.86	Joback Method
cpg	1385.41	J/mol×K	1014.54	Joback Method
cpg	1403.24	J/mol×K	1050.21	Joback Method
cpg	1419.69	J/mol×K	1085.88	Joback Method
cpg	1434.82	J/mol×K	1121.56	Joback Method
cpg	1448.69	J/mol×K	1157.23	Joback Method
dvisc	0.0004231	Pa×s	514.52	Joback Method
dvisc	0.0001730	Pa×s	585.97	Joback Method

dvisc	0.0000859	Pa×s	657.41	Joback Method
dvisc	0.0000490	Pa×s	728.86	Joback Method
dvisc	0.0000308	Pa×s	800.30	Joback Method
dvisc	0.0000210	Pa×s	871.75	Joback Method
dvisc	0.0000151	Pa×s	943.19	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=U361591&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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