Dimethylmalonic acid, pentadecyl 2-pentyl ester

Inchi: InChI=1S/C25H48O4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)25(4,5)24(2

InchiKey: CJLXWWRNQIZXQR-UHFFFAOYSA-N

Formula: C25H48O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)OC(C)CCC

Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-307.82	kJ/mol	Joback Method
hf	-1062.96	kJ/mol	Joback Method
hfus	55.14	kJ/mol	Joback Method
hvap	87.87	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	7.379		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	816.79	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	920.31	K	Joback Method
tc	1127.45	K	Joback Method
tf	503.25	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.45	J/mol×K	920.31	Joback Method
cpg	1369.31	J/mol×K	1092.93	Joback Method
cpg	1354.33	J/mol×K	1058.41	Joback Method
cpg	1338.12	J/mol×K	1023.88	Joback Method
cpg	1320.61	J/mol×K	989.36	Joback Method
cpg	1301.73	J/mol×K	954.83	Joback Method
cpg	1383.09	J/mol×K	1127.45	Joback Method
dvisc	0.0000178	Pa×s	920.31	Joback Method

dvisc	0.0000246	Pa×s	850.80	Joback Method
dvisc	0.0000362	Pa×s	781.29	Joback Method
dvisc	0.0000573	Pa×s	711.78	Joback Method
dvisc	0.0001003	Pa×s	642.27	Joback Method
dvisc	0.0002009	Pa×s	572.76	Joback Method
dvisc	0.0004880	Pa×s	503.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361590&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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