Diethylmalonic acid, decyl 2,4,4-trimethylpentyl ester

Inchi: InChI=1S/C25H48O4/c1-8-11-12-13-14-15-16-17-18-28-22(26)25(9-2,10-3)23(27)29-20-
InchiKey: LHASJMFCRWBEQB-UHFFFAOYSA-N
Formula: C25H48O4
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	-304.98	kJ/mol	Joback Method
hf	-1071.71	kJ/mol	Joback Method
hfus	47.73	kJ/mol	Joback Method
hvap	86.58	kJ/mol	Joback Method
log10ws	-7.29		Crippen Method
logp	7.092		Crippen Method
mcvol	377.990	ml/mol	McGowan Method
pc	825.74	kPa	Joback Method
rinpol	2413.00		NIST Webbook
tb	917.08	K	Joback Method
tc	1122.77	K	Joback Method
tf	505.67	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.38	J/mol×K	917.08	Joback Method
cpg	1301.42	J/mol×K	951.36	Joback Method
cpg	1320.15	J/mol×K	985.64	Joback Method
cpg	1337.62	J/mol×K	1019.92	Joback Method
cpg	1353.92	J/mol×K	1054.20	Joback Method
cpg	1369.12	J/mol×K	1088.48	Joback Method
cpg	1383.30	J/mol×K	1122.77	Joback Method
dvisc	0.0004445	Pa×s	505.67	Joback Method
dvisc	0.0001762	Pa×s	574.24	Joback Method

dvisc	0.0000850	Pa×s	642.81	Joback Method
dvisc	0.0000472	Pa×s	711.38	Joback Method
dvisc	0.0000291	Pa×s	779.94	Joback Method
dvisc	0.0000194	Pa×s	848.51	Joback Method
dvisc	0.0000137	Pa×s	917.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369482&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

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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