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

Inchi: InChI=1S/C21H40O4/c1-8-11-12-13-14-24-18(22)21(9-2,10-3)19(23)25-16-17(4)15-20(5

InchiKey: HERKBCPQYFCDHL-UHFFFAOYSA-N

Formula: C21H40O4

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-338.66	kJ/mol	Joback Method
hf	-989.15	kJ/mol	Joback Method
hfus	37.37	kJ/mol	Joback Method
hvap	77.67	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.532		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2012.00		NIST Webbook
tb	825.56	K	Joback Method
tc	1017.59	K	Joback Method
tf	460.59	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1032.28	J/mol×K	825.56	Joback Method
cpg	1115.03	J/mol×K	985.59	Joback Method
cpg	1100.54	J/mol×K	953.58	Joback Method
cpg	1085.07	J/mol×K	921.58	Joback Method
cpg	1068.57	J/mol×K	889.57	Joback Method
cpg	1050.99	J/mol×K	857.57	Joback Method
cpg	1128.59	J/mol×K	1017.59	Joback Method
dvisc	0.0000268	Pa×s	825.56	Joback Method
dvisc	0.0000376	Pa×s	764.73	Joback Method

dvisc	0.0000562	Pa×s	703.90	Joback Method
dvisc	0.0000905	Pa×s	643.08	Joback Method
dvisc	0.0001609	Pa×s	582.25	Joback Method
dvisc	0.0003271	Pa×s	521.42	Joback Method
dvisc	0.0008026	Pa×s	460.59	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=U369478&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