Diethylmalonic acid, heptyl 5-methylhex-2-yl ester

Inchi: InChI=1S/C21H40O4/c1-7-10-11-12-13-16-24-19(22)21(8-2,9-3)20(23)25-18(6)15-14-17
InchiKey: KLNAWULWJZWWNK-UHFFFAOYSA-N
Formula: C21H40O4
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)OC(C)CCC(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	-343.94	kJ/mol	Joback Method
hf	-985.68	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	78.58	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.674		Crippen Method
mcvol	321.630	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	2077.00		NIST Webbook
tb	828.35	K	Joback Method
tc	1018.59	K	Joback Method
tf	443.17	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1031.95	J/mol×K	828.35	Joback Method
cpg	1050.71	J/mol×K	860.06	Joback Method
cpg	1068.32	J/mol×K	891.76	Joback Method
cpg	1084.83	J/mol×K	923.47	Joback Method
cpg	1100.26	J/mol×K	955.18	Joback Method
cpg	1114.66	J/mol×K	986.89	Joback Method
cpg	1128.05	J/mol×K	1018.59	Joback Method
dvisc	0.0010254	Pa×s	443.17	Joback Method
dvisc	0.0003951	Pa×s	507.37	Joback Method

dvisc	0.0001886	Pa×s	571.56	Joback Method
dvisc	0.0001045	Pa×s	635.76	Joback Method
dvisc	0.0000646	Pa×s	699.96	Joback Method
dvisc	0.0000432	Pa×s	764.15	Joback Method
dvisc	0.0000308	Pa×s	828.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369299&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