Diethylmalonic acid, heptyl 3-methylphenyl ester

Inchi: InChI=1S/C21H32O4/c1-5-8-9-10-11-15-24-19(22)21(6-2,7-3)20(23)25-18-14-12-13-17(4

InchiKey: FDOZORHBKZWCSO-UHFFFAOYSA-N

Formula: C21H32O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-236.28	kJ/mol	Joback Method
hf	-750.06	kJ/mol	Joback Method
hfus	41.96	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	5.220		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1269.16	kPa	Joback Method
rinpol	2237.00		NIST Webbook
tb	860.89	K	Joback Method
tc	1066.30	K	Joback Method
tf	512.11	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.93	J/mol×K	860.89	Joback Method
cpg	954.39	J/mol×K	895.13	Joback Method
cpg	969.67	J/mol×K	929.36	Joback Method
cpg	983.83	J/mol×K	963.60	Joback Method
cpg	996.89	J/mol×K	997.83	Joback Method
cpg	1008.90	J/mol×K	1032.07	Joback Method
cpg	1019.92	J/mol×K	1066.30	Joback Method
dvisc	0.0004882	Pa×s	512.11	Joback Method
dvisc	0.0002558	Pa×s	570.24	Joback Method

dvisc	0.0001510	Pa×s	628.37	Joback Method
dvisc	0.0000975	Pa×s	686.50	Joback Method
dvisc	0.0000674	Pa×s	744.63	Joback Method
dvisc	0.0000492	Pa×s	802.76	Joback Method
dvisc	0.0000374	Pa×s	860.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370015&Units=SI

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