Diethylmalonic acid, 3-ethylphenyl octyl ester

Inchi: InChI=1S/C23H36O4/c1-5-9-10-11-12-13-17-26-21(24)23(7-3,8-4)22(25)27-20-16-14-15-
InchiKey: KZGHJLHBWQVVAX-UHFFFAOYSA-N
Formula: C23H36O4
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-219.44	kJ/mol	Joback Method
hf	-791.34	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	86.75	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.864		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2416.00		NIST Webbook
tb	906.65	K	Joback Method
tc	1114.81	K	Joback Method
tf	534.65	K	Joback Method
vc	1.252	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.41	J/mol×K	906.65	Joback Method
cpg	1075.23	J/mol×K	941.34	Joback Method
cpg	1090.81	J/mol×K	976.04	Joback Method
cpg	1105.18	J/mol×K	1010.73	Joback Method
cpg	1118.41	J/mol×K	1045.42	Joback Method
cpg	1130.55	J/mol×K	1080.12	Joback Method
cpg	1141.65	J/mol×K	1114.81	Joback Method
dvisc	0.0003857	Pa×s	534.65	Joback Method
dvisc	0.0001978	Pa×s	596.65	Joback Method

dvisc	0.0001150	Pa×s	658.65	Joback Method
dvisc	0.0000734	Pa×s	720.65	Joback Method
dvisc	0.0000503	Pa×s	782.65	Joback Method
dvisc	0.0000365	Pa×s	844.65	Joback Method
dvisc	0.0000276	Pa×s	906.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370590&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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