Diethylmalonic acid, 2-ethylphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C22H34O4/c1-7-13-18(16(5)6)25-20(23)22(9-3,10-4)21(24)26-19-15-12-11-14-

InchiKey: NWGGYTAJJQEEQT-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccccc1CC)C(C)C

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-232.74	kJ/mol	Joback Method
hf	-781.26	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	83.74	kJ/mol	Joback Method
log10ws	-6.10		Crippen Method
logp	5.329		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2160.00		NIST Webbook
tb	882.89	K	Joback Method
tc	1092.45	K	Joback Method
tf	493.38	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.81	J/mol×K	882.89	Joback Method
cpg	1015.65	J/mol×K	917.82	Joback Method
cpg	1031.21	J/mol×K	952.74	Joback Method
cpg	1045.56	J/mol×K	987.67	Joback Method
cpg	1058.74	J/mol×K	1022.60	Joback Method
cpg	1070.79	J/mol×K	1057.52	Joback Method
cpg	1081.78	J/mol×K	1092.45	Joback Method
dvisc	0.0005713	Pa×s	493.38	Joback Method
dvisc	0.0002554	Pa×s	558.30	Joback Method

dvisc	0.0001350	Pa×s	623.22	Joback Method
dvisc	0.0000805	Pa×s	688.13	Joback Method
dvisc	0.0000525	Pa×s	753.05	Joback Method
dvisc	0.0000366	Pa×s	817.97	Joback Method
dvisc	0.0000269	Pa×s	882.89	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=U370244&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