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

Inchi: InChI=1S/C22H34O4/c1-6-12-19(17(4)5)26-21(24)22(7-2,8-3)20(23)25-16-15-18-13-10-9

InchiKey: CNJRDUBABOHXLQ-UHFFFAOYSA-N

Formula: C22H34O4

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)OCCc1ccccc1)C(C)C

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-223.11	kJ/mol	Joback Method
hf	-769.79	kJ/mol	Joback Method
hfus	37.89	kJ/mol	Joback Method
hvap	83.08	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.947		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2222.00		NIST Webbook
tb	877.91	K	Joback Method
tc	1086.61	K	Joback Method
tf	480.86	K	Joback Method
vc	1.185	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	999.40	J/mol×K	877.91	Joback Method
cpg	1016.33	J/mol×K	912.69	Joback Method
cpg	1032.00	J/mol×K	947.48	Joback Method
cpg	1046.46	J/mol×K	982.26	Joback Method
cpg	1059.77	J/mol×K	1017.05	Joback Method
cpg	1071.97	J/mol×K	1051.83	Joback Method
cpg	1083.14	J/mol×K	1086.61	Joback Method
dvisc	0.0006929	Pa×s	480.86	Joback Method
dvisc	0.0002896	Pa×s	547.03	Joback Method

dvisc	0.0001461	Pa×s	613.21	Joback Method
dvisc	0.0000842	Pa×s	679.38	Joback Method
dvisc	0.0000535	Pa×s	745.56	Joback Method
dvisc	0.0000366	Pa×s	811.74	Joback Method
dvisc	0.0000265	Pa×s	877.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369549&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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