Diethylmalonic acid, 3-methoxyphenyl octyl ester

Inchi: InChI=1S/C22H34O5/c1-5-8-9-10-11-12-16-26-20(23)22(6-2,7-3)21(24)27-19-15-13-14-1

InchiKey: MZFRTNKGSFHKAG-UHFFFAOYSA-N

Formula: C22H34O5

SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(OC)c1

Mol. weight [g/mol]: 378.50

Physical Properties

Property code	Value	Unit	Source
gf	-332.86	kJ/mol	Joback Method
hf	-902.92	kJ/mol	Joback Method
hfus	45.74	kJ/mol	Joback Method
hvap	86.93	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.311		Crippen Method
mcvol	317.830	ml/mol	McGowan Method
pc	1172.83	kPa	Joback Method
rinpol	2507.00		NIST Webbook
tb	906.19	K	Joback Method
tc	1114.59	K	Joback Method
tf	545.61	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.42	J/mol×K	906.19	Joback Method
cpg	1043.46	J/mol×K	940.92	Joback Method
cpg	1058.20	J/mol×K	975.66	Joback Method
cpg	1071.67	J/mol×K	1010.39	Joback Method
cpg	1083.90	J/mol×K	1045.12	Joback Method
cpg	1094.93	J/mol×K	1079.86	Joback Method
cpg	1104.79	J/mol×K	1114.59	Joback Method
dvisc	0.0002975	Pa×s	545.61	Joback Method
dvisc	0.0001585	Pa×s	605.71	Joback Method

dvisc	0.0000946	Pa×s	665.80	Joback Method
dvisc	0.0000615	Pa×s	725.90	Joback Method
dvisc	0.0000427	Pa×s	786.00	Joback Method
dvisc	0.0000312	Pa×s	846.09	Joback Method
dvisc	0.0000238	Pa×s	906.19	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=U370875&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