Diethylmalonic acid, di(2,3-dimethylphenyl) ester

Inchi: InChI=1S/C23H28O4/c1-7-23(8-2,21(24)26-19-13-9-11-15(3)17(19)5)22(25)27-20-14-10-
InchiKey: VBXFQEIRCVQQJJ-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCC(CC)(C(=O)Oc1cccc(C)c1C)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-135.92	kJ/mol	Joback Method
hf	-589.22	kJ/mol	Joback Method
hfus	40.01	kJ/mol	Joback Method
hvap	91.01	kJ/mol	Joback Method
log10ws	-6.67		Crippen Method
logp	5.238		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1358.63	kPa	Joback Method
rinpol	2664.00		NIST Webbook
tb	948.27	K	Joback Method
tc	1178.02	K	Joback Method
tf	598.63	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.23	J/mol×K	948.27	Joback Method
cpg	968.52	J/mol×K	986.56	Joback Method
cpg	981.45	J/mol×K	1024.85	Joback Method
cpg	993.07	J/mol×K	1063.15	Joback Method
cpg	1003.42	J/mol×K	1101.44	Joback Method
cpg	1012.57	J/mol×K	1139.73	Joback Method
cpg	1020.56	J/mol×K	1178.02	Joback Method
dvisc	0.0002313	Pa×s	598.63	Joback Method
dvisc	0.0001415	Pa×s	656.90	Joback Method

dvisc	0.0000938	Pa×s	715.18	Joback Method
dvisc	0.0000661	Pa×s	773.45	Joback Method
dvisc	0.0000490	Pa×s	831.72	Joback Method
dvisc	0.0000377	Pa×s	890.00	Joback Method
dvisc	0.0000300	Pa×s	948.27	Joback Method

Sources

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=U370580&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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