Diethylmalonic acid, di(3-methylbenzyl) ester

Inchi: InChI=1S/C23H28O4/c1-5-23(6-2,21(24)26-15-19-11-7-9-17(3)13-19)22(25)27-16-20-12-8-10-18(4)14-20/h7-14H,5-6,15-16H2,1-4H3
InchiKey: QOPXANGJMHGWKZ-UHFFFAOYSA-N
Formula: C23H28O4
SMILES: CCC(CC)(C(=O)OCc1cccc(C)c1)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]: 368.47

Physical Properties

Property code	Value	Unit	Source
gf	-116.66	kJ/mol	Joback Method
hf	-566.28	kJ/mol	Joback Method
hfus	40.79	kJ/mol	Joback Method
hvap	89.68	kJ/mol	Joback Method
log10ws	-6.24		Crippen Method
logp	4.896		Crippen Method
mcvol	302.290	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	938.31	K	Joback Method
tc	1166.48	K	Joback Method
tf	573.59	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	956.39	J/mol×K	938.31	Joback Method
cpg	970.93	J/mol×K	976.34	Joback Method
cpg	984.13	J/mol×K	1014.37	Joback Method
cpg	996.08	J/mol×K	1052.39	Joback Method
cpg	1006.83	J/mol×K	1090.42	Joback Method
cpg	1016.46	J/mol×K	1128.45	Joback Method
cpg	1025.04	J/mol×K	1166.48	Joback Method
dvisc	0.0002918	Pa×s	573.59	Joback Method

dvisc	0.0001649	Pa×s	634.38	Joback Method
dvisc	0.0001029	Pa×s	695.16	Joback Method
dvisc	0.0000693	Pa×s	755.95	Joback Method
dvisc	0.0000495	Pa×s	816.74	Joback Method
dvisc	0.0000371	Pa×s	877.52	Joback Method
dvisc	0.0000288	Pa×s	938.31	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=U369319&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