

Diethylmalonic acid, 2,3-dimethylphenyl octyl ester

Inchi:	InChI=1S/C23H36O4/c1-6-9-10-11-12-13-17-26-21(24)23(7-2,8-3)22(25)27-20-16-14-15
InchiKey:	XAZJYKVLHMERCK-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-229.07	kJ/mol	Joback Method
hf	-802.81	kJ/mol	Joback Method
hfus	46.75	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.919		Crippen Method
mvol	326.050	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	911.63	K	Joback Method
tc	1120.72	K	Joback Method
tf	547.17	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.83	J/molxK	911.63	Joback Method
cpg	1074.56	J/molxK	946.48	Joback Method
cpg	1090.03	J/molxK	981.33	Joback Method
cpg	1104.29	J/molxK	1016.18	Joback Method
cpg	1117.38	J/molxK	1051.02	Joback Method
cpg	1129.34	J/molxK	1085.87	Joback Method
cpg	1140.24	J/molxK	1120.72	Joback Method
dvisc	0.0003331	Paxs	547.17	Joback Method

dvisc	0.0001795	Paxs	607.91	Joback Method
dvisc	0.0001083	Paxs	668.66	Joback Method
dvisc	0.0000710	Paxs	729.40	Joback Method
dvisc	0.0000497	Paxs	790.14	Joback Method
dvisc	0.0000366	Paxs	850.89	Joback Method
dvisc	0.0000281	Paxs	911.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370569&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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