

Diethylmalonic acid, 3-ethylphenyl octyl ester

Inchi:	InChI=1S/C23H36O4/c1-5-9-10-11-12-13-17-26-21(24)23(7-3,8-4)22(25)27-20-16-14-15
InchiKey:	KZGHJLHBWQVVAX-UHFFFAOYSA-N
Formula:	C23H36O4
SMILES:	CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(CC)c1
Mol. weight [g/mol]:	376.53

Physical Properties

Property code	Value	Unit	Source
gf	-219.44	kJ/mol	Joback Method
hf	-791.34	kJ/mol	Joback Method
hfus	47.14	kJ/mol	Joback Method
hvap	86.75	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.864		Crippen Method
mcvol	326.050	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2416.00		NIST Webbook
tb	906.65	K	Joback Method
tc	1114.81	K	Joback Method
tf	534.65	K	Joback Method
vc	1.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.41	J/molxK	906.65	Joback Method
cpg	1075.23	J/molxK	941.34	Joback Method
cpg	1090.81	J/molxK	976.04	Joback Method
cpg	1105.18	J/molxK	1010.73	Joback Method
cpg	1118.41	J/molxK	1045.42	Joback Method
cpg	1130.55	J/molxK	1080.12	Joback Method
cpg	1141.65	J/molxK	1114.81	Joback Method
dvisc	0.0003857	Paxs	534.65	Joback Method
dvisc	0.0001978	Paxs	596.65	Joback Method

dvisc	0.0001150	Paxs	658.65	Joback Method
dvisc	0.0000734	Paxs	720.65	Joback Method
dvisc	0.0000503	Paxs	782.65	Joback Method
dvisc	0.0000365	Paxs	844.65	Joback Method
dvisc	0.0000276	Paxs	906.65	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=U370590&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

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