Diethylmalonic acid, 3-methylphenyl octyl ester

Inchi: InChI=1S/C22H34O4/c1-5-8-9-10-11-12-16-25-20(23)22(6-2,7-3)21(24)26-19-15-13-14-1

InchiKey: NZGNZXPWMMHZNI-UHFFFAOYSA-N

Formula: C22H34O4

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

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-227.86	kJ/mol	Joback Method
hf	-770.70	kJ/mol	Joback Method
hfus	44.55	kJ/mol	Joback Method
hvap	84.52	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.611		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2336.00		NIST Webbook
tb	883.77	K	Joback Method
tc	1090.17	K	Joback Method
tf	523.38	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.84	J/mol×K	883.77	Joback Method
cpg	1014.47	J/mol×K	918.17	Joback Method
cpg	1029.90	J/mol×K	952.57	Joback Method
cpg	1044.16	J/mol×K	986.97	Joback Method
cpg	1057.31	J/mol×K	1021.37	Joback Method
cpg	1069.39	J/mol×K	1055.77	Joback Method
cpg	1080.45	J/mol×K	1090.17	Joback Method
dvisc	0.0004346	Pa×s	523.38	Joback Method
dvisc	0.0002253	Pa×s	583.44	Joback Method

dvisc	0.0001320	Pa×s	643.51	Joback Method
dvisc	0.0000847	Pa×s	703.57	Joback Method
dvisc	0.0000583	Pa×s	763.64	Joback Method
dvisc	0.0000424	Pa×s	823.70	Joback Method
dvisc	0.0000322	Pa×s	883.77	Joback Method

Sources

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=U370016&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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