Diethylmalonic acid, 2,3-dimethylphenyl nonyl ester

Inchi: InChI=1S/C24H38O4/c1-6-9-10-11-12-13-14-18-27-22(25)24(7-2,8-3)23(26)28-21-17-15-

InchiKey: UPLNDKZBHMBTGQ-UHFFFAOYSA-N

Formula: C24H38O4

SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cccc(C)c1C

Mol. weight [g/mol]: 390.56

Physical Properties

Property code	Value	Unit	Source
gf	-220.65	kJ/mol	Joback Method
hf	-823.45	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	89.63	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.309		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2592.00		NIST Webbook
tb	934.51	K	Joback Method
tc	1146.26	K	Joback Method
tf	558.44	K	Joback Method
vc	1.308	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.03	J/mol×K	934.51	Joback Method
cpg	1135.96	J/mol×K	969.80	Joback Method
cpg	1151.59	J/mol×K	1005.09	Joback Method
cpg	1165.95	J/mol×K	1040.38	Joback Method
cpg	1179.10	J/mol×K	1075.68	Joback Method
cpg	1191.10	J/mol×K	1110.97	Joback Method
cpg	1201.99	J/mol×K	1146.26	Joback Method
dvisc	0.0002958	Pa×s	558.44	Joback Method
dvisc	0.0001578	Pa×s	621.12	Joback Method

dvisc	0.0000944	Pa×s	683.80	Joback Method
dvisc	0.0000616	Pa×s	746.48	Joback Method
dvisc	0.0000429	Pa×s	809.15	Joback Method
dvisc	0.0000315	Pa×s	871.83	Joback Method
dvisc	0.0000241	Pa×s	934.51	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=U370570&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