Diethylmalonic acid, 2,3-dimethylphenyl hexyl ester

Inchi: InChI=1S/C21H32O4/c1-6-9-10-11-15-24-19(22)21(7-2,8-3)20(23)25-18-14-12-13-16(4)1

InchiKey: OVKXSMJZARHDMM-UHFFFAOYSA-N

Formula: C21H32O4

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

Mol. weight [g/mol]: 348.48

Physical Properties

Property code	Value	Unit	Source
gf	-245.91	kJ/mol	Joback Method
hf	-761.53	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	82.96	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.139		Crippen Method
mcvol	297.870	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2299.00		NIST Webbook
tb	865.87	K	Joback Method
tc	1072.14	K	Joback Method
tf	524.63	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.29	J/mol×K	865.87	Joback Method
cpg	953.67	J/mol×K	900.25	Joback Method
cpg	968.86	J/mol×K	934.63	Joback Method
cpg	982.91	J/mol×K	969.00	Joback Method
cpg	995.86	J/mol×K	1003.38	Joback Method
cpg	1007.75	J/mol×K	1037.76	Joback Method
cpg	1018.60	J/mol×K	1072.14	Joback Method
dvisc	0.0004181	Pa×s	524.63	Joback Method
dvisc	0.0002304	Pa×s	581.50	Joback Method

dvisc	0.0001412	Pa×s	638.38	Joback Method
dvisc	0.0000938	Pa×s	695.25	Joback Method
dvisc	0.0000662	Pa×s	752.12	Joback Method
dvisc	0.0000491	Pa×s	809.00	Joback Method
dvisc	0.0000379	Pa×s	865.87	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=U370567&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