Diethylmalonic acid, 2,3-dimethylphenyl heptyl ester

Inchi: InChI=1S/C22H34O4/c1-6-9-10-11-12-16-25-20(23)22(7-2,8-3)21(24)26-19-15-13-14-17

InchiKey: HNXYSBKZNVBCQA-UHFFFAOYSA-N

Formula: C22H34O4

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

Mol. weight [g/mol]: 362.50

Physical Properties

Property code	Value	Unit	Source
gf	-237.49	kJ/mol	Joback Method
hf	-782.17	kJ/mol	Joback Method
hfus	44.16	kJ/mol	Joback Method
hvap	85.18	kJ/mol	Joback Method
log10ws	-6.38		Crippen Method
logp	5.529		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	2395.00		NIST Webbook
tb	888.75	K	Joback Method
tc	1096.04	K	Joback Method
tf	535.90	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.23	J/mol×K	888.75	Joback Method
cpg	1013.78	J/mol×K	923.30	Joback Method
cpg	1029.11	J/mol×K	957.85	Joback Method
cpg	1043.26	J/mol×K	992.39	Joback Method
cpg	1056.29	J/mol×K	1026.94	Joback Method
cpg	1068.22	J/mol×K	1061.49	Joback Method
cpg	1079.10	J/mol×K	1096.04	Joback Method
dvisc	0.0003738	Pa×s	535.90	Joback Method
dvisc	0.0002037	Pa×s	594.71	Joback Method

dvisc	0.0001238	Pa×s	653.52	Joback Method
dvisc	0.0000817	Pa×s	712.33	Joback Method
dvisc	0.0000575	Pa×s	771.13	Joback Method
dvisc	0.0000425	Pa×s	829.94	Joback Method
dvisc	0.0000327	Pa×s	888.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370568&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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