Diethylmalonic acid, 2-chloro-5-methylphenyl heptyl ester

Inchi: InChI=1S/C21H31ClO4/c1-5-8-9-10-11-14-25-19(23)21(6-2,7-3)20(24)26-18-15-16(4)12-

InchiKey: PWFZCTAHSIVNMU-UHFFFAOYSA-N

Formula: C21H31ClO4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-257.84	kJ/mol	Joback Method
hf	-777.27	kJ/mol	Joback Method
hfus	45.77	kJ/mol	Joback Method
hvap	87.34	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.874		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1223.41	kPa	Joback Method
rinpol	2429.00		NIST Webbook
tb	903.30	K	Joback Method
tc	1114.76	K	Joback Method
tf	554.55	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.07	J/mol×K	903.30	Joback Method
cpg	979.25	J/mol×K	938.54	Joback Method
cpg	993.24	J/mol×K	973.79	Joback Method
cpg	1006.10	J/mol×K	1009.03	Joback Method
cpg	1017.85	J/mol×K	1044.27	Joback Method
cpg	1028.56	J/mol×K	1079.52	Joback Method
cpg	1038.26	J/mol×K	1114.76	Joback Method
dvisc	0.0003357	Pa×s	554.55	Joback Method
dvisc	0.0001887	Pa×s	612.67	Joback Method

dvisc	0.0001172	Pa×s	670.80	Joback Method
dvisc	0.0000785	Pa×s	728.92	Joback Method
dvisc	0.0000558	Pa×s	787.05	Joback Method
dvisc	0.0000416	Pa×s	845.17	Joback Method
dvisc	0.0000322	Pa×s	903.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370457&Units=SI

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