Dimethylmalonic acid, 4-chlorophenyl decyl ester

Inchi: InChI=1S/C21H31ClO4/c1-4-5-6-7-8-9-10-11-16-25-19(23)21(2,3)20(24)26-18-14-12-17(

InchiKey: IYGRBRODGNJUDE-UHFFFAOYSA-N

Formula: C21H31ClO4

SMILES: CCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-248.21	kJ/mol	Joback Method
hf	-765.80	kJ/mol	Joback Method
hfus	46.15	kJ/mol	Joback Method
hvap	86.68	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.955		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1236.35	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	898.32	K	Joback Method
tc	1108.90	K	Joback Method
tf	542.03	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.91	J/mol×K	898.32	Joback Method
cpg	980.17	J/mol×K	933.42	Joback Method
cpg	994.27	J/mol×K	968.51	Joback Method
cpg	1007.23	J/mol×K	1003.61	Joback Method
cpg	1019.13	J/mol×K	1038.71	Joback Method
cpg	1030.00	J/mol×K	1073.80	Joback Method
cpg	1039.89	J/mol×K	1108.90	Joback Method
dvisc	0.0003864	Pa×s	542.03	Joback Method

dvisc	0.0002073	Pa×s	601.41	Joback Method
dvisc	0.0001244	Pa×s	660.79	Joback Method
dvisc	0.0000812	Pa×s	720.17	Joback Method
dvisc	0.0000566	Pa×s	779.56	Joback Method
dvisc	0.0000415	Pa×s	838.94	Joback Method
dvisc	0.0000317	Pa×s	898.32	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=U361980&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