Diethylmalonic acid, 4-chlorobenzyl undecyl ester

Inchi: InChI=1S/C25H39ClO4/c1-4-7-8-9-10-11-12-13-14-19-29-23(27)25(5-2,6-3)24(28)30-20-
InchiKey: SLVODSQGUPTVAN-UHFFFAOYSA-N
Formula: C25H39ClO4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Cl)cc1
Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-214.53	kJ/mol	Joback Method
hf	-848.36	kJ/mol	Joback Method
hfus	56.51	kJ/mol	Joback Method
hvap	95.58	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	7.264		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinpol	2848.00		NIST Webbook
rinpol	2848.00		NIST Webbook
tb	989.84	K	Joback Method
tc	1211.90	K	Joback Method
tf	587.11	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.74	J/mol×K	989.84	Joback Method
cpg	1275.69	J/mol×K	1174.89	Joback Method
cpg	1264.51	J/mol×K	1137.88	Joback Method
cpg	1252.20	J/mol×K	1100.87	Joback Method
cpg	1238.68	J/mol×K	1063.86	Joback Method
cpg	1223.89	J/mol×K	1026.85	Joback Method
cpg	1285.80	J/mol×K	1211.90	Joback Method
dvisc	0.0000169	Pa×s	989.84	Joback Method

dvisc	0.0000223	Pa×s	922.72	Joback Method
dvisc	0.0000308	Pa×s	855.60	Joback Method
dvisc	0.0000449	Pa×s	788.47	Joback Method
dvisc	0.0000703	Pa×s	721.35	Joback Method
dvisc	0.0001205	Pa×s	654.23	Joback Method
dvisc	0.0002339	Pa×s	587.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369783&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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