Diethylmalonic acid, 3-chlorobenzyl tridecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-20-31-25(29)27(5-2,6-3)26(30)

InchiKey: UTWWYFOJWRRVJZ-UHFFFAOYSA-N

Formula: C27H43ClO4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Cl)c1

Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-197.69	kJ/mol	Joback Method
hf	-889.64	kJ/mol	Joback Method
hfus	61.69	kJ/mol	Joback Method
hvap	100.03	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.044		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	3052.00		NIST Webbook
rinpol	3052.00		NIST Webbook
tb	1035.60	K	Joback Method
tc	1269.41	K	Joback Method
tf	609.65	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.20	J/mol×K	1035.60	Joback Method
cpg	1348.97	J/mol×K	1074.57	Joback Method
cpg	1364.25	J/mol×K	1113.54	Joback Method
cpg	1378.13	J/mol×K	1152.50	Joback Method
cpg	1390.71	J/mol×K	1191.47	Joback Method
cpg	1402.08	J/mol×K	1230.44	Joback Method
cpg	1412.33	J/mol×K	1269.41	Joback Method
dvisc	0.0001793	Pa×s	609.65	Joback Method

dvisc	0.0000907	Pa×s	680.64	Joback Method
dvisc	0.0000522	Pa×s	751.63	Joback Method
dvisc	0.0000330	Pa×s	822.62	Joback Method
dvisc	0.0000225	Pa×s	893.62	Joback Method
dvisc	0.0000162	Pa×s	964.61	Joback Method
dvisc	0.0000122	Pa×s	1035.60	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=U369352&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

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