Diethylmalonic acid, 8-chlorooctyl undecyl ester

Inchi: InChI=1S/C26H49ClO4/c1-4-7-8-9-10-11-13-16-19-22-30-24(28)26(5-2,6-3)25(29)31-23-

InchiKey: JHTIJWGNSUBWPQ-UHFFFAOYSA-N

Formula: C26H49ClO4

SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 461.12

Physical Properties

Property code	Value	Unit	Source
gf	-308.89	kJ/mol	Joback Method
hf	-1094.06	kJ/mol	Joback Method
hfus	65.45	kJ/mol	Joback Method
hvap	94.87	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.989		Crippen Method
mcvol	404.320	ml/mol	McGowan Method
pc	754.74	kPa	Joback Method
rinpol	2957.00		NIST Webbook
rinpol	2957.00		NIST Webbook
tb	981.06	K	Joback Method
tc	1207.26	K	Joback Method
tf	559.44	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.20	J/mol×K	981.06	Joback Method
cpg	1460.46	J/mol×K	1169.56	Joback Method
cpg	1446.24	J/mol×K	1131.86	Joback Method
cpg	1430.68	J/mol×K	1094.16	Joback Method
cpg	1413.71	J/mol×K	1056.46	Joback Method
cpg	1395.24	J/mol×K	1018.76	Joback Method
cpg	1473.42	J/mol×K	1207.26	Joback Method
dvisc	0.0000136	Pa×s	981.06	Joback Method

dvisc	0.0000186	Pa×s	910.79	Joback Method
dvisc	0.0000266	Pa×s	840.52	Joback Method
dvisc	0.0000406	Pa×s	770.25	Joback Method
dvisc	0.0000675	Pa×s	699.98	Joback Method
dvisc	0.0001259	Pa×s	629.71	Joback Method
dvisc	0.0002745	Pa×s	559.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370757&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