Diethylmalonic acid, 8-chlorooctyl nonyl ester

Inchi: InChI=1S/C24H45ClO4/c1-4-7-8-9-11-14-17-20-28-22(26)24(5-2,6-3)23(27)29-21-18-15-
InchiKey: BLHKAHDUQJECFB-UHFFFAOYSA-N
Formula: C24H45ClO4
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 433.06

Physical Properties

Property code	Value	Unit	Source
gf	-325.73	kJ/mol	Joback Method
hf	-1052.78	kJ/mol	Joback Method
hfus	60.27	kJ/mol	Joback Method
hvap	90.42	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.209		Crippen Method
mcvol	376.140	ml/mol	McGowan Method
pc	841.13	kPa	Joback Method
rinpol	2751.00		NIST Webbook
rinpol	2751.00		NIST Webbook
tb	935.30	K	Joback Method
tc	1146.08	K	Joback Method
tf	536.90	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1248.44	J/mol×K	935.30	Joback Method
cpg	1330.16	J/mol×K	1110.95	Joback Method
cpg	1316.31	J/mol×K	1075.82	Joback Method
cpg	1301.27	J/mol×K	1040.69	Joback Method
cpg	1284.98	J/mol×K	1005.56	Joback Method
cpg	1267.40	J/mol×K	970.43	Joback Method
cpg	1342.90	J/mol×K	1146.08	Joback Method
dvisc	0.0000190	Pa×s	935.30	Joback Method

dvisc	0.0000257	Pa×s	868.90	Joback Method
dvisc	0.0000366	Pa×s	802.50	Joback Method
dvisc	0.0000556	Pa×s	736.10	Joback Method
dvisc	0.0000918	Pa×s	669.70	Joback Method
dvisc	0.0001691	Pa×s	603.30	Joback Method
dvisc	0.0003624	Pa×s	536.90	Joback Method

Sources

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=U370755&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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