Diethylmalonic acid, 2,4-dichloro-6-formylphenyl tetradecyl ester

Inchi: InChI=1S/C28H42Cl2O5/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-34-26(32)28(5-2,6-3)27

InchiKey: MSDZNBJNZVFNSJ-UHFFFAOYSA-N

Formula: C28H42Cl2O5

SMILES: CCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 529.54

Physical Properties

Property code	Value	Unit	Source
gf	-319.98	kJ/mol	Joback Method
hf	-1034.54	kJ/mol	Joback Method
hfus	69.99	kJ/mol	Joback Method
hvap	114.69	kJ/mol	Joback Method
log10ws	-9.97		Crippen Method
logp	8.762		Crippen Method
mcvol	422.550	ml/mol	McGowan Method
pc	812.14	kPa	Joback Method
rinpol	3389.00		NIST Webbook
tb	1154.53	K	Joback Method
tc	1428.30	K	Joback Method
tf	717.88	K	Joback Method
vc	1.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.14	J/mol×K	1154.53	Joback Method
cpg	1435.96	J/mol×K	1200.16	Joback Method
cpg	1447.96	J/mol×K	1245.79	Joback Method
cpg	1458.27	J/mol×K	1291.42	Joback Method
cpg	1467.02	J/mol×K	1337.04	Joback Method
cpg	1474.36	J/mol×K	1382.67	Joback Method
cpg	1480.40	J/mol×K	1428.30	Joback Method
dvisc	0.0000924	Pa×s	717.88	Joback Method
dvisc	0.0000529	Pa×s	790.65	Joback Method

dvisc	0.0000333	Pa×s	863.43	Joback Method
dvisc	0.0000226	Pa×s	936.20	Joback Method
dvisc	0.0000161	Pa×s	1008.98	Joback Method
dvisc	0.0000121	Pa×s	1081.75	Joback Method
dvisc	0.0000094	Pa×s	1154.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370074&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