Dimethylmalonic acid, 2,5-dichlorophenyl pentadecyl ester

Inchi: InChI=1S/C26H40Cl2O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-31-24(29)26(2,3)25(30

InchiKey: MFEJYOJMNTYSEP-UHFFFAOYSA-N

Formula: C26H40Cl2O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl

Mol. weight [g/mol]: 487.50

Physical Properties

Property code	Value	Unit	Source
gf	-227.67	kJ/mol	Joback Method
hf	-896.21	kJ/mol	Joback Method
hfus	62.91	kJ/mol	Joback Method
hvap	102.86	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.559		Crippen Method
mcvol	392.800	ml/mol	McGowan Method
pc	877.39	kPa	Joback Method
rinpol	3123.00		NIST Webbook
rinpol	3123.00		NIST Webbook
tb	1055.13	K	Joback Method
tc	1293.12	K	Joback Method
tf	640.82	K	Joback Method
vc	1.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1292.89	J/mol×K	1055.13	Joback Method
cpg	1355.23	J/mol×K	1253.46	Joback Method
cpg	1345.33	J/mol×K	1213.79	Joback Method
cpg	1334.24	J/mol×K	1174.13	Joback Method
cpg	1321.86	J/mol×K	1134.46	Joback Method
cpg	1308.11	J/mol×K	1094.80	Joback Method
cpg	1364.01	J/mol×K	1293.12	Joback Method
dvisc	0.0000121	Pa×s	1055.13	Joback Method

dvisc	0.0000158	Pa×s	986.08	Joback Method
dvisc	0.0000215	Pa×s	917.03	Joback Method
dvisc	0.0000307	Pa×s	847.97	Joback Method
dvisc	0.0000467	Pa×s	778.92	Joback Method
dvisc	0.0000771	Pa×s	709.87	Joback Method
dvisc	0.0001416	Pa×s	640.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363692&Units=SI

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