Diethylmalonic acid, 4-chloro-2-methylphenyl decyl ester

Inchi: InChI=1S/C24H37ClO4/c1-5-8-9-10-11-12-13-14-17-28-22(26)24(6-2,7-3)23(27)29-21-16

InchiKey: BBXQUMPKNRFZEM-UHFFFAOYSA-N

Formula: C24H37ClO4

SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 425.00

Physical Properties

Property code	Value	Unit	Source
gf	-232.58	kJ/mol	Joback Method
hf	-839.19	kJ/mol	Joback Method
hfus	53.54	kJ/mol	Joback Method
hvap	94.02	kJ/mol	Joback Method
log10ws	-7.85		Crippen Method
logp	7.044		Crippen Method
mcvol	352.380	ml/mol	McGowan Method
pc	1009.73	kPa	Joback Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook
tb	971.94	K	Joback Method
tc	1190.76	K	Joback Method
tf	588.36	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1145.42	J/mol×K	971.94	Joback Method
cpg	1161.20	J/mol×K	1008.41	Joback Method
cpg	1175.66	J/mol×K	1044.88	Joback Method
cpg	1188.86	J/mol×K	1081.35	Joback Method
cpg	1200.85	J/mol×K	1117.82	Joback Method
cpg	1211.70	J/mol×K	1154.29	Joback Method
cpg	1221.47	J/mol×K	1190.76	Joback Method
dvisc	0.0002338	Pa×s	588.36	Joback Method

dvisc	0.0001273	Pa×s	652.29	Joback Method
dvisc	0.0000773	Pa×s	716.22	Joback Method
dvisc	0.0000509	Pa×s	780.15	Joback Method
dvisc	0.0000357	Pa×s	844.08	Joback Method
dvisc	0.0000263	Pa×s	908.01	Joback Method
dvisc	0.0000202	Pa×s	971.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370114&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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