Fumaric acid, 2-chloro-5-methylphenyl dodecyl ester

Inchi: InChI=1S/C23H33ClO4/c1-3-4-5-6-7-8-9-10-11-12-17-27-22(25)15-16-23(26)28-21-18-19

InchiKey: PKAHTTPOKHAOIZ-FOCLMDBBSA-N

Formula: C23H33ClO4

SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 408.96

Physical Properties

Property code	Value	Unit	Source
gf	-163.62	kJ/mol	Joback Method
hf	-692.58	kJ/mol	Joback Method
hfus	58.56	kJ/mol	Joback Method
hvap	93.05	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.574		Crippen Method
mcvol	333.990	ml/mol	McGowan Method
pc	1097.90	kPa	Joback Method
rinpol	2973.00		NIST Webbook
rinpol	2973.00		NIST Webbook
tb	956.45	K	Joback Method
tc	1172.53	K	Joback Method
tf	569.59	K	Joback Method
vc	1.292	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1055.83	J/mol×K	956.45	Joback Method
cpg	1071.02	J/mol×K	992.46	Joback Method
cpg	1084.98	J/mol×K	1028.48	Joback Method
cpg	1097.77	J/mol×K	1064.49	Joback Method
cpg	1109.42	J/mol×K	1100.50	Joback Method
cpg	1119.99	J/mol×K	1136.51	Joback Method
cpg	1129.52	J/mol×K	1172.53	Joback Method
dvisc	0.0002810	Pa×s	569.59	Joback Method

dvisc	0.0001561	Pa×s	634.07	Joback Method
dvisc	0.0000967	Pa×s	698.54	Joback Method
dvisc	0.0000649	Pa×s	763.02	Joback Method
dvisc	0.0000464	Pa×s	827.50	Joback Method
dvisc	0.0000348	Pa×s	891.97	Joback Method
dvisc	0.0000271	Pa×s	956.45	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=U348263&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