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

Inchi: InChI=1S/C26H39ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-30-25(28)18-19-26(29)31

InchiKey: JSUKITLKOSYESH-VHEBQXMUSA-N

Formula: C26H39ClO4

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

Mol. weight [g/mol]: 451.04

Physical Properties

Property code	Value	Unit	Source
gf	-138.36	kJ/mol	Joback Method
hf	-754.50	kJ/mol	Joback Method
hfus	66.33	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-8.78		Crippen Method
logp	7.744		Crippen Method
mcvol	376.260	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	3289.00		NIST Webbook
rinpol	3289.00		NIST Webbook
tb	1025.09	K	Joback Method
tc	1255.86	K	Joback Method
tf	603.40	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1240.11	J/mol×K	1025.09	Joback Method
cpg	1256.18	J/mol×K	1063.55	Joback Method
cpg	1270.82	J/mol×K	1102.01	Joback Method
cpg	1284.09	J/mol×K	1140.48	Joback Method
cpg	1296.05	J/mol×K	1178.94	Joback Method
cpg	1306.79	J/mol×K	1217.40	Joback Method
cpg	1316.37	J/mol×K	1255.86	Joback Method
dvisc	0.0001971	Pa×s	603.40	Joback Method

dvisc	0.0001062	Pa×s	673.68	Joback Method
dvisc	0.0000644	Pa×s	743.96	Joback Method
dvisc	0.0000425	Pa×s	814.24	Joback Method
dvisc	0.0000300	Pa×s	884.53	Joback Method
dvisc	0.0000223	Pa×s	954.81	Joback Method
dvisc	0.0000172	Pa×s	1025.09	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=U348265&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