

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

Inchi:	InChI=1S/C24H35ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-18-28-23(26)16-17-24(27)29-22-19
InchiKey:	XEZKRMZPMBNLSV-WUKNDPDISA-N
Formula:	C24H35ClO4
SMILES:	CCCCCCCCCCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	422.99

Physical Properties

Property code	Value	Unit	Source
gf	-155.20	kJ/mol	Joback Method
hf	-713.22	kJ/mol	Joback Method
hfus	61.15	kJ/mol	Joback Method
hvap	95.27	kJ/mol	Joback Method
log10ws	-7.94		Crippen Method
logp	6.964		Crippen Method
mcvol	348.080	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	3083.00		NIST Webbook
rinpol	3083.00		NIST Webbook
tb	979.33	K	Joback Method
tc	1199.27	K	Joback Method
tf	580.86	K	Joback Method
vc	1.349	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.75	J/molxK	979.33	Joback Method
cpg	1132.21	J/molxK	1015.99	Joback Method
cpg	1146.38	J/molxK	1052.64	Joback Method
cpg	1159.32	J/molxK	1089.30	Joback Method
cpg	1171.08	J/molxK	1125.95	Joback Method
cpg	1181.71	J/molxK	1162.61	Joback Method
cpg	1191.26	J/molxK	1199.27	Joback Method
dvisc	0.0002504	Paxs	580.86	Joback Method

dvisc	0.0001377	Paxs	647.27	Joback Method
dvisc	0.0000846	Paxs	713.68	Joback Method
dvisc	0.0000565	Paxs	780.10	Joback Method
dvisc	0.0000402	Paxs	846.51	Joback Method
dvisc	0.0000301	Paxs	912.92	Joback Method
dvisc	0.0000234	Paxs	979.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348264&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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