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

Inchi: InChI=1S/C22H31ClO4/c1-3-4-5-6-7-8-9-10-11-16-26-21(24)14-15-22(25)27-20-17-18(2)

InchiKey: VGDMPBSGYSHRRP-CCEZHUSRSA-N

Formula: C22H31ClO4

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

Mol. weight [g/mol]: 394.93

Physical Properties

Property code	Value	Unit	Source
gf	-172.04	kJ/mol	Joback Method
hf	-671.94	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.184		Crippen Method
mcvol	319.900	ml/mol	McGowan Method
pc	1171.22	kPa	Joback Method
rinpol	2865.00		NIST Webbook
tb	933.57	K	Joback Method
tc	1146.73	K	Joback Method
tf	558.32	K	Joback Method
vc	1.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	995.47	J/mol×K	933.57	Joback Method
cpg	1058.86	J/mol×K	1111.21	Joback Method
cpg	1048.36	J/mol×K	1075.68	Joback Method
cpg	1036.81	J/mol×K	1040.15	Joback Method
cpg	1024.18	J/mol×K	1004.62	Joback Method
cpg	1010.41	J/mol×K	969.10	Joback Method
cpg	1068.36	J/mol×K	1146.73	Joback Method
dvisc	0.0000315	Pa×s	933.57	Joback Method
dvisc	0.0000402	Pa×s	871.03	Joback Method

dvisc	0.0000534	Pa×s	808.49	Joback Method
dvisc	0.0000744	Pa×s	745.94	Joback Method
dvisc	0.0001102	Pa×s	683.40	Joback Method
dvisc	0.0001765	Pa×s	620.86	Joback Method
dvisc	0.0003143	Pa×s	558.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348262&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

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