Fumaric acid, 2,4-dichlorophenyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C22H28Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-16-27-21(25)14-15-22(26)28-20-13-12

InchiKey: UFMNQBOLHZPDDZ-RICRECKTSA-N

Formula: C22H28Cl2O4

SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 427.36

Physical Properties

Property code	Value	Unit	Source
gf	-103.75	kJ/mol	Joback Method
hf	-570.46	kJ/mol	Joback Method
hfus	60.37	kJ/mol	Joback Method
hvap	95.16	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.695		Crippen Method
mcvol	327.840	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2999.00		NIST Webbook
rinpol	2999.00		NIST Webbook
tb	975.16	K	Joback Method
tc	1197.33	K	Joback Method
tf	583.16	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.88	J/mol×K	975.16	Joback Method
cpg	1004.51	J/mol×K	1012.19	Joback Method
cpg	1017.10	J/mol×K	1049.22	Joback Method
cpg	1028.73	J/mol×K	1086.25	Joback Method
cpg	1039.45	J/mol×K	1123.27	Joback Method
cpg	1049.33	J/mol×K	1160.30	Joback Method
cpg	1058.44	J/mol×K	1197.33	Joback Method
dvisc	0.0002347	Pa×s	583.16	Joback Method

dvisc	0.0001317	Pa×s	648.49	Joback Method
dvisc	0.0000821	Pa×s	713.83	Joback Method
dvisc	0.0000555	Pa×s	779.16	Joback Method
dvisc	0.0000398	Pa×s	844.49	Joback Method
dvisc	0.0000299	Pa×s	909.83	Joback Method
dvisc	0.0000234	Pa×s	975.16	Joback Method

Sources

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=U405705&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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