

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

Inchi:	InChI=1S/C22H29ClO4/c1-2-3-4-5-6-7-8-9-10-11-18-26-21(24)16-17-22(25)27-20-14-12
InchiKey:	VFXWGTMDSYDTQT-DUWBUDFISA-N
Formula:	C22H29ClO4
SMILES:	CCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	392.92

Physical Properties

Property code	Value	Unit	Source
gf	-82.19	kJ/mol	Joback Method
hf	-543.25	kJ/mol	Joback Method
hfus	56.56	kJ/mol	Joback Method
hvap	90.12	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.042		Crippen Method
mvol	315.600	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2898.00		NIST Webbook
rinpol	2898.00		NIST Webbook
tb	932.75	K	Joback Method
tc	1147.92	K	Joback Method
tf	540.72	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.20	J/molxK	932.75	Joback Method
cpg	982.90	J/molxK	968.61	Joback Method
cpg	996.56	J/molxK	1004.47	Joback Method
cpg	1009.23	J/molxK	1040.34	Joback Method
cpg	1020.99	J/molxK	1076.20	Joback Method
cpg	1031.90	J/molxK	1112.06	Joback Method
cpg	1042.02	J/molxK	1147.92	Joback Method
dvisc	0.0003311	Paxs	540.72	Joback Method

dvisc	0.0001741	Paxs	606.06	Joback Method
dvisc	0.0001037	Paxs	671.40	Joback Method
dvisc	0.0000678	Paxs	736.73	Joback Method
dvisc	0.0000474	Paxs	802.07	Joback Method
dvisc	0.0000350	Paxs	867.41	Joback Method
dvisc	0.0000270	Paxs	932.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405849&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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