

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

Inchi:	InChI=1S/C16H19ClO4/c1-3-4-5-10-20-15(18)8-9-16(19)21-14-11-12(2)6-7-13(14)17/h6-
InchiKey:	LRSWQFVWJUANNJ-CMDGGGOBGS-A-N
Formula:	C16H19ClO4
SMILES:	CCCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	310.77

Physical Properties

Property code	Value	Unit	Source
gf	-222.56	kJ/mol	Joback Method
hf	-548.10	kJ/mol	Joback Method
hfus	40.43	kJ/mol	Joback Method
hvap	77.46	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.843		Crippen Method
mvol	235.360	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rmpol	2241.00		NIST Webbook
tb	796.29	K	Joback Method
tc	1008.62	K	Joback Method
tf	490.70	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	648.45	J/molxK	796.29	Joback Method
cpg	661.84	J/molxK	831.68	Joback Method
cpg	674.28	J/molxK	867.07	Joback Method
cpg	685.80	J/molxK	902.46	Joback Method
cpg	696.40	J/molxK	937.85	Joback Method
cpg	706.13	J/molxK	973.23	Joback Method
cpg	714.98	J/molxK	1008.62	Joback Method
dvisc	0.0005682	Paxs	490.70	Joback Method
dvisc	0.0003431	Paxs	541.63	Joback Method

dvisc	0.0002260	Paxs	592.56	Joback Method
dvisc	0.0001590	Paxs	643.50	Joback Method
dvisc	0.0001178	Paxs	694.43	Joback Method
dvisc	0.0000909	Paxs	745.36	Joback Method
dvisc	0.0000725	Paxs	796.29	Joback Method

Sources

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=U348258&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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