

Fumaric acid, 2-pentyl 2,3-dichlorophenyl ester

Inchi:	InChI=1S/C15H16Cl2O4/c1-3-5-10(2)20-13(18)8-9-14(19)21-12-7-4-6-11(16)15(12)17/h
InchiKey:	BXCXMXQFABVKNS-CMDGGGOBGS-A-N
Formula:	C15H16Cl2O4
SMILES:	CCCC(C)OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]:	331.19

Physical Properties

Property code	Value	Unit	Source
gf	-245.35	kJ/mol	Joback Method
hf	-548.48	kJ/mol	Joback Method
hfus	38.52	kJ/mol	Joback Method
hvap	79.24	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.187		Crippen Method
mvol	233.510	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2224.00		NIST Webbook
rinpol	2224.00		NIST Webbook
tb	810.40	K	Joback Method
tc	1031.36	K	Joback Method
tf	494.35	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.74	J/molxK	810.40	Joback Method
cpg	629.86	J/molxK	847.23	Joback Method
cpg	641.01	J/molxK	884.05	Joback Method
cpg	651.22	J/molxK	920.88	Joback Method
cpg	660.53	J/molxK	957.71	Joback Method
cpg	668.95	J/molxK	994.53	Joback Method
cpg	676.50	J/molxK	1031.36	Joback Method
dvisc	0.0005841	Paxs	494.35	Joback Method

dvisc	0.0003420	Paxs	547.02	Joback Method
dvisc	0.0002200	Paxs	599.70	Joback Method
dvisc	0.0001520	Paxs	652.38	Joback Method
dvisc	0.0001110	Paxs	705.05	Joback Method
dvisc	0.0000847	Paxs	757.72	Joback Method
dvisc	0.0000669	Paxs	810.40	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405564&Units=SI

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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