

Fumaric acid, 2,5-dichlorophenyl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C12H8Cl4O4/c13-7-1-2-8(14)9(5-7)20-12(18)4-3-11(17)19-6-10(15)16/h1-5,10
InchiKey:	RZAIKXZEZBIHDV-ONEGZZNKSA-N
Formula:	C12H8Cl4O4
SMILES:	O=C(C=CC(=O)Oc1cc(Cl)ccc1Cl)OCC(Cl)Cl
Mol. weight [g/mol]:	358.00

Physical Properties

Property code	Value	Unit	Source
gf	-294.47	kJ/mol	Joback Method
hf	-518.04	kJ/mol	Joback Method
hfus	39.14	kJ/mol	Joback Method
hvap	81.33	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.802		Crippen Method
mcvol	215.720	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2305.00		NIST Webbook
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tb	816.62	K	Joback Method
tc	1052.51	K	Joback Method
tf	520.38	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.69	J/molxK	816.62	Joback Method
cpg	533.61	J/molxK	1013.19	Joback Method
cpg	528.23	J/molxK	973.88	Joback Method
cpg	522.08	J/molxK	934.56	Joback Method
cpg	515.11	J/molxK	895.25	Joback Method
cpg	507.33	J/molxK	855.93	Joback Method
cpg	538.23	J/molxK	1052.51	Joback Method
dvisc	0.0000765	Paxs	816.62	Joback Method

dvisc	0.0000955	Paxs	767.25	Joback Method
dvisc	0.0001228	Paxs	717.87	Joback Method
dvisc	0.0001639	Paxs	668.50	Joback Method
dvisc	0.0002291	Paxs	619.13	Joback Method
dvisc	0.0003393	Paxs	569.75	Joback Method
dvisc	0.0005416	Paxs	520.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405967&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

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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