Fumaric acid, 3-phenylpropyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C15H16Cl2O4/c16-13(17)11-21-15(19)9-8-14(18)20-10-4-7-12-5-2-1-3-6-12/h1

InchiKey: ZEOSAQHXBMFYTC-CMDGGOBGSA-N

Formula: C15H16Cl2O4

SMILES: O=C(C=CC(=O)OCC(Cl)Cl)OCCCc1ccccc1

Mol. weight [g/mol]: 331.19

Physical Properties

Property code	Value	Unit	Source
gf	-226.09	kJ/mol	Joback Method
hf	-525.54	kJ/mol	Joback Method
hfus	39.29	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.066		Crippen Method
mcvol	233.510	ml/mol	McGowan Method
pc	1977.07	kPa	Joback Method
rinpol	2319.00		NIST Webbook
rinpol	2319.00		NIST Webbook
tb	800.44	K	Joback Method
tc	1019.88	K	Joback Method
tf	469.31	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.56	J/mol×K	800.44	Joback Method
cpg	632.83	J/mol×K	837.01	Joback Method
cpg	644.14	J/mol×K	873.59	Joback Method
cpg	654.50	J/mol×K	910.16	Joback Method
cpg	663.96	J/mol×K	946.73	Joback Method
cpg	672.56	J/mol×K	983.31	Joback Method
cpg	680.33	J/mol×K	1019.88	Joback Method
dvisc	0.0008099	Pa×s	469.31	Joback Method

dvisc	0.0004275	Pa×s	524.50	Joback Method
dvisc	0.0002549	Pa×s	579.69	Joback Method
dvisc	0.0001663	Pa×s	634.88	Joback Method
dvisc	0.0001161	Pa×s	690.06	Joback Method
dvisc	0.0000855	Pa×s	745.25	Joback Method
dvisc	0.0000657	Pa×s	800.44	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=U405664&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

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