Fumaric acid, 2-phenethyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C14H14Cl2O4/c15-12(16)10-20-14(18)7-6-13(17)19-9-8-11-4-2-1-3-5-11/h1-7,

InchiKey: MQEZQDNODIEQQF-VOTSOKGWSA-N

Formula: C14H14Cl2O4

SMILES: O=C(C=CC(=O)OCC(Cl)Cl)OCCc1ccccc1

Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	-234.51	kJ/mol	Joback Method
hf	-504.90	kJ/mol	Joback Method
hfus	36.70	kJ/mol	Joback Method
hvap	75.69	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.675		Crippen Method
mcvol	219.420	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	777.56	K	Joback Method
tc	999.79	K	Joback Method
tf	458.04	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.70	J/mol×K	777.56	Joback Method
cpg	578.62	J/mol×K	814.60	Joback Method
cpg	589.58	J/mol×K	851.64	Joback Method
cpg	599.62	J/mol×K	888.68	Joback Method
cpg	608.77	J/mol×K	925.72	Joback Method
cpg	617.08	J/mol×K	962.75	Joback Method
cpg	624.57	J/mol×K	999.79	Joback Method
dvisc	0.0008947	Pa×s	458.04	Joback Method

dvisc	0.0004782	Pa×s	511.29	Joback Method
dvisc	0.0002876	Pa×s	564.55	Joback Method
dvisc	0.0001888	Pa×s	617.80	Joback Method
dvisc	0.0001326	Pa×s	671.05	Joback Method
dvisc	0.0000980	Pa×s	724.31	Joback Method
dvisc	0.0000755	Pa×s	777.56	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=U405678&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