Fumaric acid, 2-methoxyphenyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C13H12Cl2O5/c1-18-9-4-2-3-5-10(9)20-13(17)7-6-12(16)19-8-11(14)15/h2-7,1

InchiKey: ZVLDYCTWCDTEIN-VOTSOKGWSA-N

Formula: C13H12Cl2O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 319.14

Physical Properties

Property code	Value	Unit	Source
gf	-357.56	kJ/mol	Joback Method
hf	-627.95	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	76.53	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.504		Crippen Method
mcvol	211.200	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	2184.00		NIST Webbook
rinpol	2184.00		NIST Webbook
tb	782.08	K	Joback Method
tc	1006.01	K	Joback Method
tf	481.52	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.02	J/mol×K	782.08	Joback Method
cpg	548.10	J/mol×K	819.40	Joback Method
cpg	558.23	J/mol×K	856.72	Joback Method
cpg	567.42	J/mol×K	894.05	Joback Method
cpg	575.69	J/mol×K	931.37	Joback Method
cpg	583.03	J/mol×K	968.69	Joback Method
cpg	589.46	J/mol×K	1006.01	Joback Method
dvisc	0.0005828	Pa×s	481.52	Joback Method

dvisc	0.0003415	Pa×s	531.61	Joback Method
dvisc	0.0002194	Pa×s	581.71	Joback Method
dvisc	0.0001512	Pa×s	631.80	Joback Method
dvisc	0.0001100	Pa×s	681.89	Joback Method
dvisc	0.0000836	Pa×s	731.99	Joback Method
dvisc	0.0000659	Pa×s	782.08	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=U405931&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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