

Fumaric acid, 2,2-dichloroethyl nonyl ester

Inchi:	InChI=1S/C15H24Cl2O4/c1-2-3-4-5-6-7-8-11-20-14(18)9-10-15(19)21-12-13(16)17/h9-10
InchiKey:	NPEAWWXVPHOFTF-MDZDMXLPSA-N
Formula:	C15H24Cl2O4
SMILES:	CCCCCCCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	339.25

Physical Properties

Property code	Value	Unit	Source
gf	-338.50	kJ/mol	Joback Method
hf	-762.07	kJ/mol	Joback Method
hfus	45.25	kJ/mol	Joback Method
hvap	75.64	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.183		Crippen Method
mvol	257.270	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2232.00		NIST Webbook
rinpol	2232.00		NIST Webbook
tb	773.76	K	Joback Method
tc	965.92	K	Joback Method
tf	442.89	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.80	J/molxK	773.76	Joback Method
cpg	774.79	J/molxK	933.90	Joback Method
cpg	763.98	J/molxK	901.87	Joback Method
cpg	752.40	J/molxK	869.84	Joback Method
cpg	740.02	J/molxK	837.81	Joback Method
cpg	726.83	J/molxK	805.79	Joback Method
cpg	784.84	J/molxK	965.92	Joback Method
dvisc	0.0000649	Paxs	773.76	Joback Method

dvisc	0.0000858	Paxs	718.62	Joback Method
dvisc	0.0001188	Paxs	663.47	Joback Method
dvisc	0.0001746	Paxs	608.33	Joback Method
dvisc	0.0002770	Paxs	553.18	Joback Method
dvisc	0.0004867	Paxs	498.03	Joback Method
dvisc	0.0009841	Paxs	442.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348577&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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