

Fumaric acid, butyl 2-chloropropyl ester

Inchi:	InChI=1S/C11H17ClO4/c1-3-4-7-15-10(13)5-6-11(14)16-8-9(2)12/h5-6,9H,3-4,7-8H2,1-2
InchiKey:	DGWPOGSZJVYMBF-AATRIKPKSA-N
Formula:	C11H17ClO4
SMILES:	CCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]:	248.70

Physical Properties

Property code	Value	Unit	Source
gf	-360.25	kJ/mol	Joback Method
hf	-663.77	kJ/mol	Joback Method
hfus	30.70	kJ/mol	Joback Method
hvap	62.35	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.056		Crippen Method
mcvol	188.670	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinsol	1662.00		NIST Webbook
tb	644.81	K	Joback Method
tc	837.44	K	Joback Method
tf	367.89	K	Joback Method
vc	0.723	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.55	J/molxK	644.81	Joback Method
cpg	485.50	J/molxK	676.92	Joback Method
cpg	497.78	J/molxK	709.02	Joback Method
cpg	509.40	J/molxK	741.13	Joback Method
cpg	520.36	J/molxK	773.23	Joback Method
cpg	530.69	J/molxK	805.34	Joback Method
cpg	540.38	J/molxK	837.44	Joback Method
dvisc	0.0017688	Paxs	367.89	Joback Method
dvisc	0.0008896	Paxs	414.04	Joback Method

dvisc	0.0005136	Paxs	460.20	Joback Method
dvisc	0.0003277	Paxs	506.35	Joback Method
dvisc	0.0002254	Paxs	552.50	Joback Method
dvisc	0.0001643	Paxs	598.66	Joback Method
dvisc	0.0001253	Paxs	644.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348563&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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