Fumaric acid, butyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C10H14Cl2O4/c1-2-3-6-15-9(13)4-5-10(14)16-7-8(11)12/h4-5,8H,2-3,6-7H2,1H
InchiKey: DHVYZRRCEDWZEQ-SNAWJCMRSA-N
Formula: C10H14Cl2O4
SMILES: CCCCOC(=O)C=CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 269.12

Physical Properties

Property code	Value	Unit	Source
gf	-380.60	kJ/mol	Joback Method
hf	-658.87	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	64.51	kJ/mol	Joback Method
log10ws	-2.50		Crippen Method
logp	2.233		Crippen Method
mcvol	186.820	ml/mol	McGowan Method
pc	2267.57	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	659.36	K	Joback Method
tc	858.09	K	Joback Method
tf	386.54	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.08	J/mol×K	659.36	Joback Method
cpg	459.59	J/mol×K	692.48	Joback Method
cpg	470.44	J/mol×K	725.60	Joback Method
cpg	480.66	J/mol×K	758.72	Joback Method
cpg	490.25	J/mol×K	791.85	Joback Method
cpg	499.22	J/mol×K	824.97	Joback Method
cpg	507.59	J/mol×K	858.09	Joback Method
dvisc	0.0015783	Pa×s	386.54	Joback Method

dvisc	0.0008334	Pa×s	432.01	Joback Method
dvisc	0.0004970	Pa×s	477.48	Joback Method
dvisc	0.0003242	Pa×s	522.95	Joback Method
dvisc	0.0002265	Pa×s	568.42	Joback Method
dvisc	0.0001668	Pa×s	613.89	Joback Method
dvisc	0.0001282	Pa×s	659.36	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=U348575&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