2-Methoxyethyl 2,2,3,3,4,4,4-heptafluorobutanoate

Other names: 2-Methoxyethanol, heptafluorobutyrate
Inchi: InChI=1S/C7H7F7O3/c1-16-2-3-17-4(15)5(8,9)6(10,11)7(12,13)14/h2-3H2,1H3
InchiKey: IUNDPWUPTJZKAY-UHFFFAOYSA-N
Formula: C7H7F7O3
SMILES: COCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 272.12

Physical Properties

Property code	Value	Unit	Source
gf	-1686.01	kJ/mol	Joback Method
hf	-1963.85	kJ/mol	Joback Method
hfus	17.18	kJ/mol	Joback Method
hvap	33.13	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	2.009		Crippen Method
mcvol	135.190	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	779.20		NIST Webbook
rinpol	779.20		NIST Webbook
tb	443.47	K	Joback Method
tc	592.41	K	Joback Method
tf	274.43	K	Joback Method
vc	0.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.59	J/mol×K	443.47	Joback Method
cpg	338.11	J/mol×K	468.29	Joback Method
cpg	348.07	J/mol×K	493.12	Joback Method
cpg	357.49	J/mol×K	517.94	Joback Method
cpg	366.38	J/mol×K	542.77	Joback Method
cpg	374.78	J/mol×K	567.59	Joback Method
cpg	382.69	J/mol×K	592.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352014&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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