

Butanoic acid, heptafluoro-, ethyl ester

Other names:	Butyric acid, heptafluoro-, ethyl ester Ethyl heptafluorobutyrate Ethyl perfluorobutyrate Heptafluoro-n-butyric acid ethyl ester Heptafluorobutyric acid ethyl ester 2,2,3,3,4,4,4-Heptafluoro-butyric acid ethyl ester Ethyl heptafluorobutanoate
Inchi:	InChI=1S/C6H5F7O2/c1-2-15-3(14)4(7,8)5(9,10)6(11,12)13/h2H2,1H3
InchiKey:	JVHJRIQPDBCRRE-UHFFFAOYSA-N
Formula:	C6H5F7O2
SMILES:	CCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	242.09
CAS:	356-27-4

Physical Properties

Property code	Value	Unit	Source
gf	-1589.43	kJ/mol	Joback Method
hf	-1810.99	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	28.50	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.382		Crippen Method
mcvol	115.230	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	398.17	K	Joback Method
tc	546.44	K	Joback Method
tf	240.93	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.37	J/mol×K	398.17	Joback Method
cpg	273.51	J/mol×K	422.88	Joback Method

cpg	283.06	J/mol×K	447.59	Joback Method
cpg	292.04	J/mol×K	472.31	Joback Method
cpg	300.47	J/mol×K	497.02	Joback Method
cpg	308.38	J/mol×K	521.73	Joback Method
cpg	315.79	J/mol×K	546.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C356274&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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