Heptafluorobutanoic acid, methyl ester

Other names:	Butyric acid, heptafluoro-, methyl ester
	Heptafluorobutyric acid methyl ester
	Methyl heptafluorobutyrate
	Methyl perfluorobutyrate
	Methyl heptafluorobutanoate
	Heptafluorobutanoic acid, methyl ester
	2,2,3,3,4,4,4-Heptafluoro-butyric acid methyl ester
Inchi:	InChI=1S/C5H3F7O2/c1-14-2(13)3(6,7)4(8,9)5(10,11)12/h1H3
InchiKey:	MRPUVAKBXDBGJQ-UHFFFAOYSA-N
Formula:	C5H3F7O2
SMILES:	COC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	228.06

Physical Properties

Property code	Value	Unit	Source
hf	-1871.45	kJ/mol	Cheméo Relay (1.0)
hfus	10.81	kJ/mol	Joback Method
hvap	40.93	kJ/mol	Cheméo Relay (1.0)
ie	11.51	eV	Cheméo Relay (1.0)
logp	1.992		Crippen Method
mcvol	101.140	ml/mol	McGowan Method
rinpol	483.00		NIST Webbook
rinpol	482.60		NIST Webbook
rinpol	483.00		NIST Webbook
tb	353.00	K	NIST Webbook
tb	353.20	K	NIST Webbook
tf	191.40 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.73	J/mol×K	375.29	Joback Method
cpg	234.98	J/mol×K	399.97	Joback Method
cpg	243.68	J/mol×K	424.65	Joback Method

cpg	251.83	J/mol×K	449.33	Joback Method
cpg	259.47	J/mol×K	474.00	Joback Method
cpg	266.61	J/mol×K	498.68	Joback Method
cpg	273.27	J/mol×K	523.36	Joback Method
hfust	11.77	kJ/mol	191.40	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C356241&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point