Methacrylic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

Other names: Heptafluorobutyl methacrylate
1H,1H-Heptafluorobutyl methacrylate
2-Propenoic acid, 2-methyl-, 2,2,3,3,4,4,4-heptafluorobutyl ester
2,2,3,3,4,4,4-heptafluorobutyl methacrylate

Inchi: InChI=1S/C8H7F7O2/c1-4(2)5(16)17-3-6(9,10)7(11,12)8(13,14)15/h1,3H2,2H3

InchiKey: VIEHKBXCWMMOOU-UHFFFAOYSA-N

Formula: C8H7F7O2

SMILES: C=C(C)C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 268.13

CAS: 13695-31-3

Physical Properties

Property code	Value	Unit	Source
gf	-1493.30	kJ/mol	Joback Method
hf	-1736.63	kJ/mol	Joback Method
hfus	15.99	kJ/mol	Joback Method
hvap	32.36	kJ/mol	Joback Method
log10ws	-3.18		Crippen Method
logp	2.939		Crippen Method
mcvol	139.110	ml/mol	McGowan Method
pc	2161.32	kPa	Joback Method
tb	440.49	K	Joback Method
tc	593.82	K	Joback Method
tf	247.75	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.39	J/mol×K	440.49	Joback Method
cpg	339.75	J/mol×K	466.05	Joback Method
cpg	350.42	J/mol×K	491.60	Joback Method
cpg	360.43	J/mol×K	517.16	Joback Method
cpg	369.82	J/mol×K	542.71	Joback Method

cpg	378.60	J/mol×K	568.27	Joback Method
cpg	386.82	J/mol×K	593.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	328.00	K	6.70	NIST Webbook

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=C13695313&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume