

Heptafluorobutyl acrylate

Other names:	Heptafluorobutyl acrylate 2-Propenoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester 2,2,3,3,4,4,4-heptafluorobutyl acrylate
Inchi:	InChI=1S/C7H5F7O2/c1-2-4(15)16-3-5(8,9)6(10,11)7(12,13)14/h2H,1,3H2
InchiKey:	PLXOUIVCSUBZIX-UHFFFAOYSA-N
Formula:	C7H5F7O2
SMILES:	C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	254.10

Physical Properties

Property code	Value	Unit	Source
af	0.4894		Cheméo Relay (1.0)
hf	-1803.79	kJ/mol	Cheméo Relay (1.0)
hfus	14.71	kJ/mol	Joback Method
hvap	45.51	kJ/mol	Cheméo Relay (1.0)
ie	11.15	eV	Cheméo Relay (1.0)
log10ws	-3.34		Cheméo Relay (1.0)
logp	2.549		Crippen Method
mcvol	125.020	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
tb	388.25	K	Cheméo Relay (1.0)
tc	522.90	K	Cheméo Relay (1.0)
tf	212.96	K	Cheméo Relay (1.0)
vc	0.460	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	287.52	J/mol×K	417.73	Joback Method
cpg	297.98	J/mol×K	442.89	Joback Method
cpg	307.80	J/mol×K	468.05	Joback Method
cpg	317.00	J/mol×K	493.21	Joback Method
cpg	325.61	J/mol×K	518.37	Joback Method
cpg	333.66	J/mol×K	543.53	Joback Method

cpg

341.18

J/mol×K

568.69

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	330.60	K	4.00	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C424646&Units=SI>

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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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