

2-Propenoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl

Other names:
ester

2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Pentadecafluorooctyl acrylate

1H,1H-Pentadecafluorooctyl acrylate

Inchi: InChI=1S/C11H5F15O2/c1-2-4(27)28-3-5(12,13)6(14,15)7(16,17)8(18,19)9(20,21)10(22,

InchiKey: YSQGYEYXKXGAQA-UHFFFAOYSA-N

Formula: C11H5F15O2

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

Mol. weight [g/mol]: 454.13

CAS: 307-98-2

Physical Properties

Property code	Value	Unit	Source
gf	-3006.61	kJ/mol	Joback Method
hf	-3392.64	kJ/mol	Joback Method
hfus	20.05	kJ/mol	Joback Method
hvap	27.24	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.090		Crippen Method
mvol	195.540	ml/mol	McGowan Method
pc	1343.73	kPa	Joback Method
tb	490.49	K	Joback Method
tc	622.85	K	Joback Method
tf	309.92	K	Joback Method
vc	0.850	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.34	J/mol×K	490.49	Joback Method
cpg	550.94	J/mol×K	512.55	Joback Method
cpg	562.67	J/mol×K	534.61	Joback Method
cpg	573.57	J/mol×K	556.67	Joback Method
cpg	583.67	J/mol×K	578.73	Joback Method
cpg	593.03	J/mol×K	600.79	Joback Method
cpg	601.68	J/mol×K	622.85	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.50 ± 1.50	K	8.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C307982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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