

Propanoyl fluoride, 2,3,3,3-tetrafluoro-2-[1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]-

Other names:

Propionyl fluoride, tetrafluoro-2-[hexafluoro-2-(heptafluoropropoxy)propoxy]-

Propionyl fluoride,

2,3,3,3-tetrafluoro-2-[1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]-

Perfluoro-(2,5-dimethyl-3,6-dioxanonanal)

2,3,3,3-tetrafluoro-2-[1,1,2,3,3,3-hexafluoro-2-(heptafluoropropoxy)propoxy]propionyl fluoride

Perfluoro-2,5-dimethyl-3,6-dioxanonanal

Inchi: InChI=1S/C9F18O3/c10-1(28)2(11,5(15,16)17)29-9(26,27)4(14,7(21,22)23)30-8(24,25)3

InchiKey: YSIGVPOSKQLNTO-UHFFFAOYSA-N

Formula: C9F18O3

SMILES: O=C(F)C(F)(OC(F)(F)C(F)(OC(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]: 498.07

CAS: 2641-34-1

Physical Properties

Property code	Value	Unit	Source
gf	-3797.88	kJ/mol	Joback Method
hf	-4206.09	kJ/mol	Joback Method
hfus	19.17	kJ/mol	Joback Method
hvap	22.12	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	5.355		Crippen Method
mcvol	182.840	ml/mol	McGowan Method
pc	1360.63	kPa	Joback Method
tb	387.00 ± 1.00	K	NIST Webbook
tc	587.18	K	Joback Method
tf	315.56	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.24	J/molxK	465.05	Joback Method
cpg	528.74	J/molxK	485.41	Joback Method
cpg	539.46	J/molxK	505.76	Joback Method
cpg	549.43	J/molxK	526.12	Joback Method

cpg	558.69	J/mol×K	546.47	Joback Method
cpg	567.26	J/mol×K	566.83	Joback Method
cpg	575.18	J/mol×K	587.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2641341&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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