

Triacetyl pentafluoropropionate

Other names:	Triacetyl 2,2,3,3,3-pentafluoropropanoate 1-Triacetyl, pentafluoropropionate
Inchi:	InChI=1S/C33H61F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	FQGLWEGVMMMDANK-UHFFFAOYSA-N
Formula:	C33H61F5O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	584.83

Physical Properties

Property code	Value	Unit	Source
gf	-975.31	kJ/mol	Joback Method
hf	-1967.30	kJ/mol	Joback Method
hfus	84.58	kJ/mol	Joback Method
hvap	91.53	kJ/mol	Joback Method
log10ws	-13.48		Crippen Method
logp	12.670		Crippen Method
mcvol	492.120	ml/mol	McGowan Method
pc	487.95	kPa	Joback Method
rinpol	3157.00		NIST Webbook
tb	1020.62	K	Joback Method
tc	1316.19	K	Joback Method
tf	541.62	K	Joback Method
vc	1.976	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1781.66	J/mol×K	1020.62	Joback Method
cpg	1813.24	J/mol×K	1069.88	Joback Method
cpg	1842.41	J/mol×K	1119.14	Joback Method
cpg	1869.53	J/mol×K	1168.41	Joback Method
cpg	1894.94	J/mol×K	1217.67	Joback Method
cpg	1918.99	J/mol×K	1266.93	Joback Method
cpg	1942.04	J/mol×K	1316.19	Joback Method

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=U351800&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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