

Triacetyl heptafluorobutyrate

Other names:	Triacetyl 2,2,3,3,4,4,4-heptafluorobutanoate 1-Triacontanol, heptafluorobutyrate Triacetyl perfluorobutyrate
Inchi:	InChI=1S/C34H61F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	SYHLYSKOBILJEH-UHFFFAOYSA-N
Formula:	C34H61F7O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	634.84

Physical Properties

Property code	Value	Unit	Source
gf	-1353.67	kJ/mol	Joback Method
hf	-2388.91	kJ/mol	Joback Method
hfus	85.92	kJ/mol	Joback Method
hvap	90.83	kJ/mol	Joback Method
log10ws	-14.21		Crippen Method
logp	13.305		Crippen Method
mcvol	509.750	ml/mol	McGowan Method
pc	453.85	kPa	Joback Method
rinpol	3177.90		NIST Webbook
tb	1038.81	K	Joback Method
tc	1361.76	K	Joback Method
tf	556.49	K	Joback Method
vc	2.057	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1861.31	J/mol×K	1038.81	Joback Method
cpg	1895.55	J/mol×K	1092.64	Joback Method
cpg	1927.41	J/mol×K	1146.46	Joback Method
cpg	1957.43	J/mol×K	1200.29	Joback Method
cpg	1986.18	J/mol×K	1254.11	Joback Method
cpg	2014.18	J/mol×K	1307.94	Joback Method

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=U351832&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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