

Heptafluorobutyric acid, undecyl ester

Other names:	Undecyl heptafluorobutyrate
Inchi:	InChI=1S/C15H23F7O2/c1-2-3-4-5-6-7-8-9-10-11-24-12(23)13(16,17)14(18,19)15(20,21)
InchiKey:	BAMRUWAHGSFKKX-UHFFFAOYSA-N
Formula:	C15H23F7O2
SMILES:	CCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	368.33
CAS:	959103-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-1513.65	kJ/mol	Joback Method
hf	-1996.75	kJ/mol	Joback Method
hfus	36.71	kJ/mol	Joback Method
hvap	48.53	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.893		Crippen Method
mcvol	242.040	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpol	1386.00		NIST Webbook
rinpol	1392.80		NIST Webbook
tb	604.09	K	Joback Method
tc	754.43	K	Joback Method
tf	342.36	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.52	J/mol×K	604.09	Joback Method
cpg	699.86	J/mol×K	629.15	Joback Method
cpg	714.42	J/mol×K	654.20	Joback Method
cpg	728.25	J/mol×K	679.26	Joback Method
cpg	741.37	J/mol×K	704.31	Joback Method
cpg	753.82	J/mol×K	729.37	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=C959103743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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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