Heptafluorobutyric acid, n-hexyl ester

Other names:	Hexyl heptafluorobutyrate
	Hexyl 2,2,3,3,4,4,4-heptafluorobutanoate
	1-Hexanol, heptafluorobutyrate
	Hexyl perfluorobutyrate
	2,2,3,3,4,4,4-Heptafluoro-butyric acid hexyl ester
	Butanoic acid, heptafluoro, hexyl ester
	Hexyl heptafluorobutanoate
	Heptafluorobutanoic acid, hexyl ester
	Heptafluorobutyric acid, hexyl ester
Inchi:	InChI=1S/C10H13F7O2/c1-2-3-4-5-6-19-7(18)8(11,12)9(13,14)10(15,16)17/h2-6H2,1H3
InchiKey:	UCZXOGFHGJONAJ-UHFFFAOYSA-N
Formula:	C10H13F7O2
SMILES:	CCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	298.20
CAS:	336-65-2

Physical Properties

Property code	Value	Unit	Source
gf	-1555.75	kJ/mol	Joback Method
hf	-1893.55	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	37.40	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.943		Crippen Method
mcvol	171.590	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	943.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	926.20		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	936.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	920.00		NIST Webbook
ripol	923.00		NIST Webbook
ripol	907.00		NIST Webbook
tb	489.69	K	Joback Method
tc	637.76	K	Joback Method

tf	286.01	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.88	J/mol×K	489.69	Joback Method
cpg	446.81	J/mol×K	514.37	Joback Method
cpg	459.05	J/mol×K	539.05	Joback Method
cpg	470.64	J/mol×K	563.72	Joback Method
cpg	481.61	J/mol×K	588.40	Joback Method
cpg	491.97	J/mol×K	613.08	Joback Method
cpg	501.76	J/mol×K	637.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C336652&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ripol:	Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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