

Propyl perfluoroheptanoate

Other names:	2,2,3,3,4,4,5,5,6,6,7,7,7-Tridecafluoro-heptanoic acid propyl ester
Inchi:	InChI=1S/C10H7F13O2/c1-2-3-25-4(24)5(11,12)6(13,14)7(15,16)8(17,18)9(19,20)10(21,
InchiKey:	TWMBCWLVFGAURH-UHFFFAOYSA-N
Formula:	C10H7F13O2
SMILES:	CCCOC(=O)C(F)(F)C(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]:	406.14

Physical Properties

Property code	Value	Unit	Source
gf	-2716.09	kJ/mol	Joback Method
hf	-3096.46	kJ/mol	Joback Method
hfus	20.00	kJ/mol	Joback Method
hvap	28.61	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.678		Crippen Method
mcvol	182.210	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	807.00		NIST Webbook
rinpol	807.20		NIST Webbook
rinpol	807.00		NIST Webbook
tb	475.62	K	Joback Method
tc	609.60	K	Joback Method
tf	296.81	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.47	J/molxK	475.62	Joback Method
cpg	503.18	J/molxK	497.95	Joback Method
cpg	515.08	J/molxK	520.28	Joback Method
cpg	526.20	J/molxK	542.61	Joback Method
cpg	536.58	J/molxK	564.94	Joback Method
cpg	546.26	J/molxK	587.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R70254&Units=SI

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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