2,2,3,3,4,4,5,5,6,6,6-Undecafluoro- hexanoic acid hexyl ester

Other names: Hexyl perfluorohexanoate

Inchi: InChI=1S/C12H13F11O2/c1-2-3-4-5-6-25-7(24)8(13,14)9(15,16)10(17,18)11(19,20)12(21

InchiKey: TXJKATBVTOHLTD-UHFFFAOYSA-N

Formula: C12H13F11O2

SMILES: CCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 398.21

Physical Properties

Property code	Value	Unit	Source
gf	-2312.47	kJ/mol	Joback Method
hf	-2736.77	kJ/mol	Joback Method
hfus	26.43	kJ/mol	Joback Method
hvap	35.99	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.213		Crippen Method
mcvol	206.850	ml/mol	McGowan Method
pc	1347.68	kPa	Joback Method
rinpol	1030.50		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
tb	526.07	K	Joback Method
tc	665.85	K	Joback Method
tf	315.75	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.75	J/mol×K	526.07	Joback Method
cpg	581.28	J/mol×K	549.37	Joback Method
cpg	594.01	J/mol×K	572.66	Joback Method
cpg	605.99	J/mol×K	595.96	Joback Method
cpg	617.24	J/mol×K	619.26	Joback Method
cpg	627.81	J/mol×K	642.55	Joback Method

cpg	637.73	J/mol×K	665.85	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=R70147&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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