

Pentafluoropropanamide, N-(2-ethylhexyl)-

Inchi:	InChI=1S/C11H18F5NO/c1-3-5-6-8(4-2)7-17-9(18)10(12,13)11(14,15)16/h8H,3-7H2,1-2H
InchiKey:	QODLOCKHLXCIMQ-UHFFFAOYSA-N
Formula:	C11H18F5NO
SMILES:	CCCCC(CC)CNC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	275.26

Physical Properties

Property code	Value	Unit	Source
gf	-968.60	kJ/mol	Joback Method
hf	-1332.81	kJ/mol	Joback Method
hfus	27.99	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.517		Crippen Method
mvol	186.250	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1190.00		NIST Webbook
rinpol	1190.00		NIST Webbook
tb	544.57	K	Joback Method
tc	703.62	K	Joback Method
tf	309.11	K	Joback Method
vc	0.754	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.44	J/molxK	544.57	Joback Method
cpg	503.59	J/molxK	571.08	Joback Method
cpg	516.99	J/molxK	597.59	Joback Method
cpg	529.67	J/molxK	624.09	Joback Method
cpg	541.68	J/molxK	650.60	Joback Method
cpg	553.03	J/molxK	677.11	Joback Method
cpg	563.77	J/molxK	703.62	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=U407336&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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