

Pentafluoropropanamide, N-heptyl-N-octyl-

Inchi: InChI=1S/C18H32F5NO/c1-3-5-7-9-11-13-15-24(14-12-10-8-6-4-2)16(25)17(19,20)18(21)
InchiKey: DMTPCEJIUXLIPI-UHFFFAOYSA-N
Formula: C18H32F5NO
SMILES: CCCCCCCN(CCCCCC)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 373.44

Physical Properties

Property code	Value	Unit	Source
gf	-885.83	kJ/mol	Joback Method
hf	-1457.95	kJ/mol	Joback Method
hfus	47.57	kJ/mol	Joback Method
hvap	57.77	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	6.344		Crippen Method
mvol	284.880	ml/mol	McGowan Method
pc	1059.64	kPa	Joback Method
rinpol	1803.00		NIST Webbook
rinpol	1803.00		NIST Webbook
tb	667.44	K	Joback Method
tc	824.39	K	Joback Method
tf	382.81	K	Joback Method
vc	1.135	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	842.74	J/molxK	667.44	Joback Method
cpg	860.35	J/molxK	693.60	Joback Method
cpg	877.09	J/molxK	719.76	Joback Method
cpg	893.00	J/molxK	745.92	Joback Method
cpg	908.12	J/molxK	772.07	Joback Method
cpg	922.51	J/molxK	798.23	Joback Method
cpg	936.20	J/molxK	824.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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