

Heptafluorobutanamide, N-heptyl-N-octyl-

Inchi:	InChI=1S/C19H32F7NO/c1-3-5-7-9-11-13-15-27(14-12-10-8-6-4-2)16(28)17(20,21)18(22)
InchiKey:	FOZMLBKFOAORCN-UHFFFAOYSA-N
Formula:	C19H32F7NO
SMILES:	CCCCCCCCN(CCCCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	423.45

Physical Properties

Property code	Value	Unit	Source
gf	-1264.19	kJ/mol	Joback Method
hf	-1879.56	kJ/mol	Joback Method
hfus	48.90	kJ/mol	Joback Method
hvap	57.07	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.979		Crippen Method
mcvol	302.510	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinsol	1822.00		NIST Webbook
tb	685.63	K	Joback Method
tc	842.63	K	Joback Method
tf	397.68	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.31	J/molxK	685.63	Joback Method
cpg	935.88	J/molxK	711.80	Joback Method
cpg	952.53	J/molxK	737.96	Joback Method
cpg	968.32	J/molxK	764.13	Joback Method
cpg	983.30	J/molxK	790.29	Joback Method
cpg	997.52	J/molxK	816.46	Joback Method
cpg	1011.03	J/molxK	842.63	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=U308275&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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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