

Pentafluoropropanamide, N,N-diheptyl-

Inchi:	InChI=1S/C17H30F5NO/c1-3-5-7-9-11-13-23(14-12-10-8-6-4-2)15(24)16(18,19)17(20,21
InchiKey:	DPBPRAWXPOTFQD-UHFFFAOYSA-N
Formula:	C17H30F5NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	359.42

Physical Properties

Property code	Value	Unit	Source
gf	-894.25	kJ/mol	Joback Method
hf	-1437.31	kJ/mol	Joback Method
hfus	44.98	kJ/mol	Joback Method
hvap	55.55	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	5.953		Crippen Method
mcvol	270.790	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	1713.00		NIST Webbook
tb	644.56	K	Joback Method
tc	799.65	K	Joback Method
tf	371.54	K	Joback Method
vc	1.079	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.68	J/mol×K	644.56	Joback Method
cpg	802.87	J/mol×K	670.41	Joback Method
cpg	819.21	J/mol×K	696.26	Joback Method
cpg	834.74	J/mol×K	722.11	Joback Method
cpg	849.51	J/mol×K	747.95	Joback Method
cpg	863.55	J/mol×K	773.80	Joback Method
cpg	876.91	J/mol×K	799.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308513&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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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