

Pentafluoropropanamide, N,N-dioctyl-

Inchi:	InChI=1S/C19H34F5NO/c1-3-5-7-9-11-13-15-25(16-14-12-10-8-6-4-2)17(26)18(20,21)19
InchiKey:	YEHCLLQKNLKEQR-UHFFFAOYSA-N
Formula:	C19H34F5NO
SMILES:	CCCCCCCCN(CCCCCCCC)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	387.47

Physical Properties

Property code	Value	Unit	Source
gf	-877.41	kJ/mol	Joback Method
hf	-1478.59	kJ/mol	Joback Method
hfus	50.16	kJ/mol	Joback Method
hvap	60.00	kJ/mol	Joback Method
log10ws	-7.10		Crippen Method
logp	6.734		Crippen Method
mcvol	298.970	ml/mol	McGowan Method
pc	996.39	kPa	Joback Method
rinpol	1897.00		NIST Webbook
tb	690.32	K	Joback Method
tc	849.66	K	Joback Method
tf	394.08	K	Joback Method
vc	1.192	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.85	J/mol×K	690.32	Joback Method
cpg	918.91	J/mol×K	716.88	Joback Method
cpg	936.06	J/mol×K	743.43	Joback Method
cpg	952.37	J/mol×K	769.99	Joback Method
cpg	967.87	J/mol×K	796.55	Joback Method
cpg	982.61	J/mol×K	823.11	Joback Method
cpg	996.64	J/mol×K	849.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308515&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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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