

Heptafluorobutanamide, N,N-dioctyl-

Inchi:	InChI=1S/C20H34F7NO/c1-3-5-7-9-11-13-15-28(16-14-12-10-8-6-4-2)17(29)18(21,22)19
InchiKey:	FKEGZVROYCXESK-UHFFFAOYSA-N
Formula:	C20H34F7NO
SMILES:	CCCCCCCCN(CCCCCCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	437.48

Physical Properties

Property code	Value	Unit	Source
gf	-1255.77	kJ/mol	Joback Method
hf	-1900.20	kJ/mol	Joback Method
hfus	51.49	kJ/mol	Joback Method
hvap	59.30	kJ/mol	Joback Method
log10ws	-7.83		Crippen Method
logp	7.369		Crippen Method
mcvol	316.600	ml/mol	McGowan Method
pc	899.10	kPa	Joback Method
rinpol	1914.00		NIST Webbook
tb	708.51	K	Joback Method
tc	868.87	K	Joback Method
tf	408.95	K	Joback Method
vc	1.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.05	J/mol×K	708.51	Joback Method
cpg	995.10	J/mol×K	735.24	Joback Method
cpg	1012.20	J/mol×K	761.96	Joback Method
cpg	1028.42	J/mol×K	788.69	Joback Method
cpg	1043.80	J/mol×K	815.42	Joback Method
cpg	1058.41	J/mol×K	842.14	Joback Method
cpg	1072.31	J/mol×K	868.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308276&Units=SI

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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