N,N-di-(n-Undecyl)heptafluorobutanamide

Other names: Heptafluorobutanamide, N,N-diundecyl-
Inchi: InChI=1S/C26H46F7NO/c1-3-5-7-9-11-13-15-17-19-21-34(22-20-18-16-14-12-10-8-6-4-2
InchiKey: LEYMXDNGRHCLNZ-UHFFFAOYSA-N
Formula: C26H46F7NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 521.64
CAS: 120219-49-0

Physical Properties

Property code	Value	Unit	Source
gf	-1205.25	kJ/mol	Joback Method
hf	-2024.04	kJ/mol	Joback Method
hfus	67.03	kJ/mol	Joback Method
hvap	72.65	kJ/mol	Joback Method
log10ws	-10.34		Crippen Method
logp	9.710		Crippen Method
mcvol	401.140	ml/mol	McGowan Method
pc	653.77	kPa	Joback Method
rinpol	2478.00		NIST Webbook
tb	845.79	K	Joback Method
tc	1042.94	K	Joback Method
tf	476.57	K	Joback Method
vc	1.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1346.70	J/mol×K	845.79	Joback Method
cpg	1369.04	J/mol×K	878.65	Joback Method
cpg	1390.13	J/mol×K	911.51	Joback Method
cpg	1410.09	J/mol×K	944.36	Joback Method
cpg	1429.03	J/mol×K	977.22	Joback Method
cpg	1447.09	J/mol×K	1010.08	Joback Method
cpg	1464.39	J/mol×K	1042.94	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120219490&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
mcvol:	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