2,2,3,3,3-Pentafluoro-N-[2-(2,2,3,3,3-pentafluoropr

Inchi: InChI=1S/C12H6F10N2O2/c13-9(14,11(17,18)19)7(25)23-5-3-1-2-4-6(5)24-8(26)10(15,1
InchiKey: PCMJGLAEBCNKMH-UHFFFAOYSA-N
Formula: C12H6F10N2O2
SMILES: O=C(Nc1ccccc1NC(=O)C(F)(F)C(F)(F)F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 400.17

Physical Properties

Property code	Value	Unit	Source
gf	-1862.86	kJ/mol	Joback Method
hf	-2180.27	kJ/mol	Joback Method
hfus	35.03	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.959		Crippen Method
mcvol	196.980	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
tb	693.48	K	Joback Method
tc	872.51	K	Joback Method
tf	484.70	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.84	J/mol×K	693.48	Joback Method
cpg	588.17	J/mol×K	723.32	Joback Method
cpg	596.67	J/mol×K	753.16	Joback Method
cpg	604.42	J/mol×K	782.99	Joback Method
cpg	611.50	J/mol×K	812.83	Joback Method
cpg	617.97	J/mol×K	842.67	Joback Method
cpg	623.92	J/mol×K	872.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373042&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
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
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