2,2,3,3,4,4,4-Heptafluoro-N-[4-[4-(2,2,3,3,4,4,4-hept

Inchi: InChI=1S/C20H10F14N2O3/c21-15(22,17(25,26)19(29,30)31)13(37)35-9-1-5-11(6-2-9)3
InchiKey: KFAJHDFIPWBVRA-UHFFFAOYSA-N
Formula: C20H10F14N2O3
SMILES: O=C(Nc1ccc(Oc2ccc(NC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc2)cc1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 592.28

Physical Properties

Property code	Value	Unit	Source
gf	-2571.28	kJ/mol	Joback Method
hf	-3054.49	kJ/mol	Joback Method
hfus	48.08	kJ/mol	Joback Method
hvap	75.55	kJ/mol	Joback Method
log10ws	-7.77		Crippen Method
logp	7.022		Crippen Method
mcvol	298.890	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2295.00		NIST Webbook
rinpol	2295.00		NIST Webbook
tb	921.22	K	Joback Method
tc	1128.04	K	Joback Method
tf	643.23	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	966.43	J/mol×K	921.22	Joback Method
cpg	975.40	J/mol×K	955.69	Joback Method
cpg	983.81	J/mol×K	990.16	Joback Method
cpg	991.83	J/mol×K	1024.63	Joback Method
cpg	999.63	J/mol×K	1059.10	Joback Method
cpg	1007.38	J/mol×K	1093.57	Joback Method
cpg	1015.24	J/mol×K	1128.04	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=U373019&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