Benzamide, pentafluoro-N-(pentafluorobenzoyl)-N-hept-2-yl-

Inchi: InChI=1S/C21H15F10NO2/c1-3-4-5-6-7(2)32(20(33)8-10(22)14(26)18(30)15(27)11(8)23)

InchiKey: RMXPTMQXWDOHHZ-UHFFFAOYSA-N

Formula: C21H15F10NO2

SMILES: CCCCCC(C)N(C(=O)c1c(F)c(F)c(F)c(F)c1F)C(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 503.33

Physical Properties

Property code	Value	Unit	Source
gf	-1843.14	kJ/mol	Joback Method
hf	-2242.42	kJ/mol	Joback Method
hfus	67.83	kJ/mol	Joback Method
hvap	80.49	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	6.329		Crippen Method
mcvol	290.050	ml/mol	McGowan Method
pc	1082.06	kPa	Joback Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook
tb	895.48	K	Joback Method
tc	1096.55	K	Joback Method
tf	627.70	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	888.92	J/mol×K	895.48	Joback Method
cpg	900.73	J/mol×K	928.99	Joback Method
cpg	911.58	J/mol×K	962.50	Joback Method
cpg	921.48	J/mol×K	996.02	Joback Method
cpg	930.46	J/mol×K	1029.53	Joback Method
cpg	938.56	J/mol×K	1063.04	Joback Method
cpg	945.79	J/mol×K	1096.55	Joback Method

Sources

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=U407958&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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