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

Inchi: InChI=1S/C16H10F14N2O2/c17-11(18,13(21,22)15(25,26)27)9(33)31-5-7-1-2-8(4-3-7)6-

InchiKey: JPWSUODUKNKFBM-UHFFFAOYSA-N

Formula: C16H10F14N2O2

SMILES: O=C(NCc1ccc(CNC(=O)C(F)(F)C(F)(F)C(F)(F)F)cc1)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 528.24

Physical Properties

Property code	Value	Unit	Source
gf	-2602.74	kJ/mol	Joback Method
hf	-3064.77	kJ/mol	Joback Method
hfus	42.88	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	4.585		Crippen Method
mcvol	260.420	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	1802.00		NIST Webbook
tb	775.62	K	Joback Method
tc	952.82	K	Joback Method
tf	536.98	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	823.53	J/mol×K	775.62	Joback Method
cpg	833.31	J/mol×K	805.15	Joback Method
cpg	842.30	J/mol×K	834.69	Joback Method
cpg	850.59	J/mol×K	864.22	Joback Method
cpg	858.30	J/mol×K	893.75	Joback Method
cpg	865.52	J/mol×K	923.28	Joback Method
cpg	872.38	J/mol×K	952.82	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=U372969&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