3-(Heptafluorobutyrylthio)benzoyl chloride

Inchi: InChI=1S/C11H4ClF7O2S/c12-7(20)5-2-1-3-6(4-5)22-8(21)9(13,14)10(15,16)11(17,18)19
InchiKey: BPOKCLDWSBNTME-UHFFFAOYSA-N
Formula: C11H4ClF7O2S
SMILES: O=C(Cl)c1cccc(SC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1
Mol. weight [g/mol]: 368.65

Physical Properties

Property code	Value	Unit	Source
gf	-1447.28	kJ/mol	Joback Method
hf	-1643.36	kJ/mol	Joback Method
hfus	28.74	kJ/mol	Joback Method
hvap	58.11	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.517		Crippen Method
mcvol	186.210	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1434.00		NIST Webbook
tb	681.89	K	Joback Method
tc	889.93	K	Joback Method
tf	428.24	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	477.19	J/mol×K	681.89	Joback Method
cpg	486.12	J/mol×K	716.56	Joback Method
cpg	494.12	J/mol×K	751.24	Joback Method
cpg	501.29	J/mol×K	785.91	Joback Method
cpg	507.70	J/mol×K	820.59	Joback Method
cpg	513.44	J/mol×K	855.26	Joback Method
cpg	518.60	J/mol×K	889.93	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=U375148&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