Heptafluorobutyric acid, 3,5-dimethylphenyl ester

Inchi: InChI=1S/C12H9F7O2/c1-6-3-7(2)5-8(4-6)21-9(20)10(13,14)11(15,16)12(17,18)19/h3-5H

InchiKey: KGUHSZWVKYJMGB-UHFFFAOYSA-N

Formula: C12H9F7O2

SMILES: Cc1cc(C)cc(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)c1

Mol. weight [g/mol]: 318.19

Physical Properties

Property code	Value	Unit	Source
gf	-1445.76	kJ/mol	Joback Method
hf	-1721.24	kJ/mol	Joback Method
hfus	22.20	kJ/mol	Joback Method
hvap	45.45	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	4.042		Crippen Method
mcvol	176.010	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	863.00		NIST Webbook
rinpol	863.00		NIST Webbook
tb	572.09	K	Joback Method
tc	750.82	K	Joback Method
tf	360.01	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.76	J/mol×K	572.09	Joback Method
cpg	473.22	J/mol×K	601.88	Joback Method
cpg	484.80	J/mol×K	631.67	Joback Method
cpg	495.57	J/mol×K	661.45	Joback Method
cpg	505.56	J/mol×K	691.24	Joback Method
cpg	514.83	J/mol×K	721.03	Joback Method
cpg	523.43	J/mol×K	750.82	Joback Method

Sources

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=U307629&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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