Pentafluoropropanoic acid, 2-naphthyl ester

Inchi: InChI=1S/C13H7F5O2/c14-12(15,13(16,17)18)11(19)20-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey: SFLRHHHTTLFFRX-UHFFFAOYSA-N
Formula: C13H7F5O2
SMILES: O=C(Oc1ccc2ccccc2c1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 290.19

Physical Properties

Property code	Value	Unit	Source
gf	-934.28	kJ/mol	Joback Method
hf	-1138.37	kJ/mol	Joback Method
hfus	23.46	kJ/mol	Joback Method
hvap	51.59	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.943		Crippen Method
mcvol	167.100	ml/mol	McGowan Method
pc	2388.85	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
tb	613.66	K	Joback Method
tc	818.23	K	Joback Method
tf	387.86	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.25	J/mol×K	613.66	Joback Method
cpg	444.22	J/mol×K	647.76	Joback Method
cpg	455.19	J/mol×K	681.85	Joback Method
cpg	465.23	J/mol×K	715.95	Joback Method
cpg	474.43	J/mol×K	750.04	Joback Method
cpg	482.85	J/mol×K	784.14	Joback Method
cpg	490.59	J/mol×K	818.23	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=U308007&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