Heptafluorobutyric acid, 2-naphthyl ester

Other names: 2-Naphthol, heptafluorobutanoate
Inchi: InChI=1S/C14H7F7O2/c15-12(16,13(17,18)14(19,20)21)11(22)23-10-6-5-8-3-1-2-4-9(8)7
InchiKey: FGDZFPRIFAOLGT-UHFFFAOYSA-N
Formula: C14H7F7O2
SMILES: O=C(Oc1ccc2ccccc2c1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 340.19

Physical Properties

Property code	Value	Unit	Source
gf	-1312.64	kJ/mol	Joback Method
hf	-1559.98	kJ/mol	Joback Method
hfus	24.79	kJ/mol	Joback Method
hvap	50.88	kJ/mol	Joback Method
log10ws	-5.72		Crippen Method
logp	4.578		Crippen Method
mcvol	184.730	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1404.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	631.85	K	Joback Method
tc	826.93	K	Joback Method
tf	402.73	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	500.55	J/mol×K	631.85	Joback Method
cpg	512.40	J/mol×K	664.36	Joback Method
cpg	523.21	J/mol×K	696.88	Joback Method
cpg	533.09	J/mol×K	729.39	Joback Method
cpg	542.12	J/mol×K	761.90	Joback Method
cpg	550.38	J/mol×K	794.42	Joback Method
cpg	557.98	J/mol×K	826.93	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=U307631&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