1-Naphthoic acid, pentafluorophenyl ester

Inchi: InChI=1S/C17H7F5O2/c18-11-12(19)14(21)16(15(22)13(11)20)24-17(23)10-7-3-5-8-4-1-
InchiKey: VJEQRCMOOXFTRW-UHFFFAOYSA-N
Formula: C17H7F5O2
SMILES: O=C(Oc1c(F)c(F)c(F)c(F)c1F)c1cccc2ccccc12
Mol. weight [g/mol]: 338.23

Physical Properties

Property code	Value	Unit	Source
gf	-842.02	kJ/mol	Joback Method
hf	-1024.25	kJ/mol	Joback Method
hfus	40.74	kJ/mol	Joback Method
hvap	68.67	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	4.755		Crippen Method
mcvol	199.700	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
rinpol	2065.00		NIST Webbook
tb	763.22	K	Joback Method
tc	975.77	K	Joback Method
tf	517.12	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.09	J/mol×K	763.22	Joback Method
cpg	545.89	J/mol×K	798.64	Joback Method
cpg	555.90	J/mol×K	834.07	Joback Method
cpg	565.14	J/mol×K	869.49	Joback Method
cpg	573.65	J/mol×K	904.92	Joback Method
cpg	581.47	J/mol×K	940.34	Joback Method
cpg	588.63	J/mol×K	975.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355687&Units=SI
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

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