2,3,4-Trifluorobenzoic acid, 2-naphthyl ester

Inchi: InChI=1S/C17H9F3O2/c18-14-8-7-13(15(19)16(14)20)17(21)22-12-6-5-10-3-1-2-4-11(10
InchiKey: LFBGPSYEVZXCKE-UHFFFAOYSA-N
Formula: C17H9F3O2
SMILES: O=C(Oc1ccc2ccccc2c1)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 302.25

Physical Properties

Property code	Value	Unit	Source
gf	-433.14	kJ/mol	Joback Method
hf	-609.09	kJ/mol	Joback Method
hfus	35.36	kJ/mol	Joback Method
hvap	68.98	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.476		Crippen Method
mcvol	196.160	ml/mol	McGowan Method
pc	2284.95	kPa	Joback Method
rinpol	2165.00		NIST Webbook
tb	754.72	K	Joback Method
tc	982.47	K	Joback Method
tf	490.90	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	522.49	J/mol×K	754.72	Joback Method
cpg	534.56	J/mol×K	792.68	Joback Method
cpg	545.67	J/mol×K	830.64	Joback Method
cpg	555.88	J/mol×K	868.60	Joback Method
cpg	565.25	J/mol×K	906.55	Joback Method
cpg	573.84	J/mol×K	944.51	Joback Method
cpg	581.71	J/mol×K	982.47	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=U308037&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