3-Trifluoromethylbenzoic acid, 2-naphthyl ester

Inchi: InChI=1S/C18H11F3O2/c19-18(20,21)15-7-3-6-14(10-15)17(22)23-16-9-8-12-4-1-2-5-13

InchiKey: GGUXZFJQGVPWCD-UHFFFAOYSA-N

Formula: C18H11F3O2

SMILES: O=C(Oc1ccc2ccccc2c1)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 316.27

Physical Properties

Property code	Value	Unit	Source
gf	-402.62	kJ/mol	Joback Method
hf	-615.54	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	68.59	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	5.078		Crippen Method
mcvol	210.250	ml/mol	McGowan Method
pc	2185.64	kPa	Joback Method
rinpol	2156.00		NIST Webbook
rinpol	2156.00		NIST Webbook
tb	764.41	K	Joback Method
tc	998.28	K	Joback Method
tf	479.55	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.59	J/mol×K	764.41	Joback Method
cpg	593.54	J/mol×K	803.39	Joback Method
cpg	605.38	J/mol×K	842.37	Joback Method
cpg	616.23	J/mol×K	881.34	Joback Method
cpg	626.19	J/mol×K	920.32	Joback Method
cpg	635.37	J/mol×K	959.30	Joback Method
cpg	643.89	J/mol×K	998.28	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=U307683&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