4-Fluoro-2-trifluoromethylbenzamide, N-(1-naphthyl)-

Inchi: InChI=1S/C18H11F4NO/c19-12-8-9-14(15(10-12)18(20,21)22)17(24)23-16-7-3-5-11-4-1-
InchiKey: VQHMZLGFEUPRLC-UHFFFAOYSA-N
Formula: C18H11F4NO
SMILES: O=C(Nc1cccc2ccccc12)c1ccc(F)cc1C(F)(F)F
Mol. weight [g/mol]: 333.28

Physical Properties

Property code	Value	Unit	Source
gf	-412.67	kJ/mol	Joback Method
hf	-637.43	kJ/mol	Joback Method
hfus	37.91	kJ/mol	Joback Method
hvap	72.46	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	5.250		Crippen Method
mcvol	216.130	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2392.00		NIST Webbook
rinpol	2392.00		NIST Webbook
tb	796.41	K	Joback Method
tc	1023.20	K	Joback Method
tf	523.09	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	612.14	J/mol×K	796.41	Joback Method
cpg	624.04	J/mol×K	834.21	Joback Method
cpg	635.00	J/mol×K	872.01	Joback Method
cpg	645.14	J/mol×K	909.81	Joback Method
cpg	654.56	J/mol×K	947.60	Joback Method
cpg	663.39	J/mol×K	985.40	Joback Method
cpg	671.75	J/mol×K	1023.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358097&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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