3-Fluoro-4-trifluoromethylbenzoic acid, 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C18H8Cl2F4O2/c19-13-8-14(20)16(11-4-2-1-3-10(11)13)26-17(25)9-5-6-12(15

InchiKey: NTZPMSQPTUBHLA-UHFFFAOYSA-N

Formula: C18H8Cl2F4O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c2ccccc12)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 403.15

Physical Properties

Property code	Value	Unit	Source
gf	-650.18	kJ/mol	Joback Method
hf	-877.54	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	6.524		Crippen Method
mcvol	236.500	ml/mol	McGowan Method
pc	1885.44	kPa	Joback Method
rinpol	2453.00		NIST Webbook
rinpol	2453.00		NIST Webbook
tb	853.48	K	Joback Method
tc	1085.89	K	Joback Method
tf	577.54	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.74	J/mol×K	853.48	Joback Method
cpg	635.53	J/mol×K	892.22	Joback Method
cpg	644.51	J/mol×K	930.95	Joback Method
cpg	652.75	J/mol×K	969.69	Joback Method
cpg	660.34	J/mol×K	1008.42	Joback Method
cpg	667.39	J/mol×K	1047.16	Joback Method
cpg	673.97	J/mol×K	1085.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357360&Units=SI

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