2,5-Di(trifluoromethyl)benzoic acid, 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C19H8Cl2F6O2/c20-14-8-15(21)16(11-4-2-1-3-10(11)14)29-17(28)12-7-9(18(2

InchiKey: WKTSUNBLHUOBON-UHFFFAOYSA-N

Formula: C19H8Cl2F6O2

SMILES: O=C(Oc1c(Cl)cc(Cl)c2ccccc12)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 453.16

Physical Properties

Property code	Value	Unit	Source
gf	-1028.54	kJ/mol	Joback Method
hf	-1299.15	kJ/mol	Joback Method
hfus	42.95	kJ/mol	Joback Method
hvap	77.82	kJ/mol	Joback Method
log10ws	-8.94		Crippen Method
logp	7.403		Crippen Method
mcvol	254.130	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	2347.00		NIST Webbook
rinpol	2347.00		NIST Webbook
tb	871.67	K	Joback Method
tc	1096.05	K	Joback Method
tf	592.41	K	Joback Method
vc	1.014	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.41	J/mol×K	871.67	Joback Method
cpg	705.84	J/mol×K	909.07	Joback Method
cpg	714.54	J/mol×K	946.46	Joback Method
cpg	722.62	J/mol×K	983.86	Joback Method
cpg	730.19	J/mol×K	1021.25	Joback Method
cpg	737.36	J/mol×K	1058.65	Joback Method
cpg	744.25	J/mol×K	1096.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357375&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

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