2,5-Di(trifluoromethyl)benzoic acid, nonyl ester

Inchi: InChI=1S/C18H22F6O2/c1-2-3-4-5-6-7-8-11-26-16(25)14-12-13(17(19,20)21)9-10-15(14

InchiKey: UYQHNMVCSRXLFH-UHFFFAOYSA-N

Formula: C18H22F6O2

SMILES: CCCCCCCCCOC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 384.36

Physical Properties

Property code	Value	Unit	Source
gf	-1203.27	kJ/mol	Joback Method
hf	-1640.22	kJ/mol	Joback Method
hfus	42.08	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Joback Method
log10ws	-7.27		Crippen Method
logp	6.632		Crippen Method
mcvol	258.780	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	1751.00		NIST Webbook
rinpol	1751.00		NIST Webbook
tb	713.33	K	Joback Method
tc	887.66	K	Joback Method
tf	424.62	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.33	J/mol×K	713.33	Joback Method
cpg	776.32	J/mol×K	742.39	Joback Method
cpg	790.45	J/mol×K	771.44	Joback Method
cpg	803.75	J/mol×K	800.50	Joback Method
cpg	816.27	J/mol×K	829.55	Joback Method
cpg	828.05	J/mol×K	858.61	Joback Method
cpg	839.13	J/mol×K	887.66	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=U338942&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