4-(Trifluoromethyl)benzoic acid, undec-2-enyl ester

Inchi: InChI=1S/C19H25F3O2/c1-2-3-4-5-6-7-8-9-10-15-24-18(23)16-11-13-17(14-12-16)19(20

InchiKey: OLIIAMXKDUPTEY-MDZDMXLPSA-N

Formula: C19H25F3O2

SMILES: CCCCCCCCC=CCOC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 342.40

Physical Properties

Property code	Value	Unit	Source
gf	-523.41	kJ/mol	Joback Method
hf	-935.09	kJ/mol	Joback Method
hfus	43.43	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.169		Crippen Method
mcvol	263.260	ml/mol	McGowan Method
pc	1328.10	kPa	Joback Method
rinpol	2017.00		NIST Webbook
rinpol	2017.00		NIST Webbook
tb	740.81	K	Joback Method
tc	927.72	K	Joback Method
tf	414.10	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.01	J/mol×K	740.81	Joback Method
cpg	785.09	J/mol×K	771.96	Joback Method
cpg	800.23	J/mol×K	803.11	Joback Method
cpg	814.49	J/mol×K	834.27	Joback Method
cpg	827.91	J/mol×K	865.42	Joback Method
cpg	840.56	J/mol×K	896.57	Joback Method
cpg	852.47	J/mol×K	927.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299446&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