3-Trifluoromethylbenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C21H27F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-26-20(25)18-14-13-15-19(17-18
InchiKey: SQKBUNFJYIWWGF-UHFFFAOYSA-N
Formula: C21H27F3O2
SMILES: CCCCCCCCCCC#CCOC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 368.43

Physical Properties

Property code	Value	Unit	Source
gf	-383.99	kJ/mol	Joback Method
hf	-821.29	kJ/mol	Joback Method
hfus	51.53	kJ/mol	Joback Method
hvap	72.84	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.396		Crippen Method
mcvol	287.140	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	791.41	K	Joback Method
tc	986.06	K	Joback Method
tf	547.82	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	860.49	J/mol×K	791.41	Joback Method
cpg	877.00	J/mol×K	823.85	Joback Method
cpg	892.50	J/mol×K	856.29	Joback Method
cpg	907.03	J/mol×K	888.74	Joback Method
cpg	920.65	J/mol×K	921.18	Joback Method
cpg	933.41	J/mol×K	953.62	Joback Method
cpg	945.36	J/mol×K	986.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299328&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