2,6-Difluorobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H26F2O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-24-20(23)19-17(21)14-13-15-18
InchiKey: DAUUIJNEUYPKOC-UHFFFAOYSA-N
Formula: C20H26F2O2
SMILES: CCCCCCCCCCC#CCOC(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-210.07	kJ/mol	Joback Method
hf	-607.26	kJ/mol	Joback Method
hfus	52.89	kJ/mol	Joback Method
hvap	73.39	kJ/mol	Joback Method
log10ws	-7.20		Crippen Method
logp	5.656		Crippen Method
mcvol	271.280	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2307.00		NIST Webbook
tb	777.47	K	Joback Method
tc	972.24	K	Joback Method
tf	546.06	K	Joback Method
vc	1.069	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.02	J/mol×K	777.47	Joback Method
cpg	809.45	J/mol×K	809.93	Joback Method
cpg	824.91	J/mol×K	842.39	Joback Method
cpg	839.43	J/mol×K	874.85	Joback Method
cpg	853.03	J/mol×K	907.31	Joback Method
cpg	865.75	J/mol×K	939.78	Joback Method
cpg	877.60	J/mol×K	972.24	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=U292589&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