3-Trifluoromethylbenzoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H19F3O2/c1-3-4-5-6-8-12(2)21-15(20)13-9-7-10-14(11-13)16(17,18)19/h6-

InchiKey: CURIZVLIDWVEPQ-SOFGYWHQSA-N

Formula: C16H19F3O2

SMILES: CCCCC=CC(C)OC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 300.32

Physical Properties

Property code	Value	Unit	Source
gf	-551.11	kJ/mol	Joback Method
hf	-878.45	kJ/mol	Joback Method
hfus	32.14	kJ/mol	Joback Method
hvap	59.13	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.997		Crippen Method
mcvol	220.990	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1607.00		NIST Webbook
tb	671.73	K	Joback Method
tc	864.38	K	Joback Method
tf	365.29	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.56	J/mol×K	671.73	Joback Method
cpg	619.90	J/mol×K	703.84	Joback Method
cpg	634.30	J/mol×K	735.95	Joback Method
cpg	647.81	J/mol×K	768.05	Joback Method
cpg	660.47	J/mol×K	800.16	Joback Method
cpg	672.33	J/mol×K	832.27	Joback Method
cpg	683.46	J/mol×K	864.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299323&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