trans-3-Trifluoromethylcinnamic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C15H11F3O2/c1-2-3-4-10-20-14(19)9-8-12-6-5-7-13(11-12)15(16,17)18/h1,3-9

InchiKey: CNVWOAKTWOKNJV-UCNKFEGYSA-N

Formula: C15H11F3O2

SMILES: C#CC=CCOC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 280.24

Physical Properties

Property code	Value	Unit	Source
gf	-253.80	kJ/mol	Joback Method
hf	-443.41	kJ/mol	Joback Method
hfus	36.25	kJ/mol	Joback Method
hvap	57.11	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.451		Crippen Method
mcvol	194.000	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
rinpol	1749.00		NIST Webbook
rinpol	1749.00		NIST Webbook
tb	643.57	K	Joback Method
tc	853.82	K	Joback Method
tf	410.91	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.28	J/mol×K	643.57	Joback Method
cpg	498.27	J/mol×K	678.61	Joback Method
cpg	510.31	J/mol×K	713.65	Joback Method
cpg	521.47	J/mol×K	748.69	Joback Method
cpg	531.84	J/mol×K	783.74	Joback Method
cpg	541.49	J/mol×K	818.78	Joback Method
cpg	550.51	J/mol×K	853.82	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=U299412&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