trans-3-Trifluoromethylcinnamic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H15F3O2/c1-3-6-14(4-2)21-15(20)10-9-12-7-5-8-13(11-12)16(17,18)19/h5
InchiKey: CTKLGNPYFDQMQP-MDZDMXLPSA-N
Formula: C16H15F3O2
SMILES: CC#CC(CC)OC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 296.28

Physical Properties

Property code	Value	Unit	Source
gf	-348.31	kJ/mol	Joback Method
hf	-606.15	kJ/mol	Joback Method
hfus	35.26	kJ/mol	Joback Method
hvap	61.28	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.064		Crippen Method
mcvol	212.390	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	680.73	K	Joback Method
tc	892.74	K	Joback Method
tf	471.39	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.61	J/mol×K	680.73	Joback Method
cpg	575.31	J/mol×K	716.07	Joback Method
cpg	589.01	J/mol×K	751.40	Joback Method
cpg	601.77	J/mol×K	786.74	Joback Method
cpg	613.65	J/mol×K	822.07	Joback Method
cpg	624.71	J/mol×K	857.41	Joback Method
cpg	635.01	J/mol×K	892.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299413&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