trans-3-Trifluoromethylcinnamic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C18H21F3O2/c1-3-4-5-6-8-14(2)23-17(22)12-11-15-9-7-10-16(13-15)18(19,20

InchiKey: WGSNWDBLWAUYTH-ZTUQJBCJSA-N

Formula: C18H21F3O2

SMILES: CCCCC=CC(C)OC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 326.35

Physical Properties

Property code	Value	Unit	Source
gf	-454.05	kJ/mol	Joback Method
hf	-802.51	kJ/mol	Joback Method
hfus	37.52	kJ/mol	Joback Method
hvap	63.54	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.397		Crippen Method
mcvol	244.870	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	1928.00		NIST Webbook
tb	721.65	K	Joback Method
tc	917.27	K	Joback Method
tf	382.75	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.00	J/mol×K	721.65	Joback Method
cpg	705.48	J/mol×K	754.25	Joback Method
cpg	720.00	J/mol×K	786.86	Joback Method
cpg	733.62	J/mol×K	819.46	Joback Method
cpg	746.42	J/mol×K	852.06	Joback Method
cpg	758.47	J/mol×K	884.66	Joback Method
cpg	769.82	J/mol×K	917.27	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=U299414&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