trans-3-(Trifluoromethyl)cinnamic acid, pentyl ester

Inchi: InChI=1S/C15H17F3O2/c1-2-3-4-10-20-14(19)9-8-12-6-5-7-13(11-12)15(16,17)18/h5-9,1

InchiKey: AKOQLJKRQZZNGF-CMDGGOBGSA-N

Formula: C15H17F3O2

SMILES: CCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 286.29

Physical Properties

Property code	Value	Unit	Source
gf	-557.09	kJ/mol	Joback Method
hf	-852.53	kJ/mol	Joback Method
hfus	33.07	kJ/mol	Joback Method
hvap	57.29	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.452		Crippen Method
mcvol	206.900	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1725.00		NIST Webbook
tb	649.29	K	Joback Method
tc	840.65	K	Joback Method
tf	369.02	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	551.47	J/mol×K	649.29	Joback Method
cpg	566.14	J/mol×K	681.18	Joback Method
cpg	579.92	J/mol×K	713.08	Joback Method
cpg	592.85	J/mol×K	744.97	Joback Method
cpg	604.97	J/mol×K	776.86	Joback Method
cpg	616.33	J/mol×K	808.75	Joback Method
cpg	626.99	J/mol×K	840.65	Joback Method

Sources

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=U299869&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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