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

Inchi: InChI=1S/C17H21F3O2/c1-2-3-4-5-6-12-22-16(21)11-10-14-8-7-9-15(13-14)17(18,19)20
InchiKey: CZOIQZJKDFRADG-ZHACJKMWSA-N
Formula: C17H21F3O2
SMILES: CCCCCCCOC(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 314.34

Physical Properties

Property code	Value	Unit	Source
gf	-540.25	kJ/mol	Joback Method
hf	-893.81	kJ/mol	Joback Method
hfus	38.25	kJ/mol	Joback Method
hvap	61.74	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	5.232		Crippen Method
mcvol	235.080	ml/mol	McGowan Method
pc	1535.46	kPa	Joback Method
rinpol	1870.00		NIST Webbook
tb	695.05	K	Joback Method
tc	883.30	K	Joback Method
tf	391.56	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.91	J/mol×K	695.05	Joback Method
cpg	673.34	J/mol×K	726.43	Joback Method
cpg	687.86	J/mol×K	757.80	Joback Method
cpg	701.51	J/mol×K	789.18	Joback Method
cpg	714.34	J/mol×K	820.55	Joback Method
cpg	726.40	J/mol×K	851.93	Joback Method
cpg	737.74	J/mol×K	883.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299871&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