trans-(3-Trifluoromethyl)cinnamic acid, 1-adamantylmethyl ester

Inchi: InChI=1S/C21H23F3O2/c22-21(23,24)18-3-1-2-14(9-18)4-5-19(25)26-13-20-10-15-6-16(

InchiKey: ANIWTKAOBMFSNQ-SNAWJCMRSA-N

Formula: C21H23F3O2

SMILES: O=C(C=Cc1cccc(C(F)(F)F)c1)OCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 364.40

Physical Properties

Property code	Value	Unit	Source
gf	-349.62	kJ/mol	Joback Method
hf	-769.23	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	5.478		Crippen Method
mcvol	258.860	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2393.60		NIST Webbook
tb	806.63	K	Joback Method
tc	1028.71	K	Joback Method
tf	506.60	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	838.74	J/mol×K	806.63	Joback Method
cpg	857.88	J/mol×K	843.64	Joback Method
cpg	876.48	J/mol×K	880.66	Joback Method
cpg	894.78	J/mol×K	917.67	Joback Method
cpg	913.06	J/mol×K	954.68	Joback Method
cpg	931.56	J/mol×K	991.70	Joback Method
cpg	950.55	J/mol×K	1028.71	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=U292262&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