trans-(3-trifluoromethyl)cinnamic acid, 2-(1-adamantyl)ethyl ester

Inchi: InChI=1S/C22H25F3O2/c23-22(24,25)19-3-1-2-15(11-19)4-5-20(26)27-7-6-21-12-16-8-17(13-21)10-18(9-16)14-21/h1-4,11,16-18H,5-10,12-14H2/b5-4+

InchiKey: XKDTWQBLOXEVMG-SNAWJCMRSA-N

Formula: C22H25F3O2

SMILES: O=C(/C=C/c1cccc(C(F)(F)F)c1)OCCC12CC3CC(CC(C3)C1)C2

Mol. weight [g/mol]: 378.43

Physical Properties

Property code	Value	Unit	Source
hfus	38.28	kJ/mol	Joback Method
ie	9.12	eV	Cheméo Relay (1.0)
logp	5.868		Crippen Method
mcvol	272.950	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.91	J/mol×K	829.51	Joback Method
cpg	917.52	J/mol×K	866.13	Joback Method
cpg	936.69	J/mol×K	902.75	Joback Method
cpg	955.67	J/mol×K	939.37	Joback Method
cpg	974.72	J/mol×K	975.99	Joback Method
cpg	994.08	J/mol×K	1012.60	Joback Method
cpg	1014.01	J/mol×K	1049.22	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292263&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume