trans-Cinnamamide, n-heptyl-n-octyl-3-trifluoromethyl-

Inchi: InChI=1S/C25H38F3NO/c1-3-5-7-9-11-13-20-29(19-12-10-8-6-4-2)24(30)18-17-22-15-14

InchiKey: BQDWRCAUWXEUTQ-ISLYRVAYSA-N

Formula: C25H38F3NO

SMILES: CCCCCCCCN(CCCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 425.57

Physical Properties

Property code	Value	Unit	Source
gf	-257.11	kJ/mol	Joback Method
hf	-859.18	kJ/mol	Joback Method
hfus	60.81	kJ/mol	Joback Method
hvap	79.18	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.878		Crippen Method
mcvol	351.910	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	2725.00		NIST Webbook
rinpol	2725.00		NIST Webbook
tb	868.11	K	Joback Method
tc	1063.72	K	Joback Method
tf	491.96	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.20	J/mol×K	868.11	Joback Method
cpg	1155.83	J/mol×K	900.71	Joback Method
cpg	1173.44	J/mol×K	933.31	Joback Method
cpg	1190.13	J/mol×K	965.92	Joback Method
cpg	1205.98	J/mol×K	998.52	Joback Method
cpg	1221.10	J/mol×K	1031.12	Joback Method
cpg	1235.57	J/mol×K	1063.72	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=U308075&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

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