

trans-Cinnamamide, N,N-dibutyl-3-trifluoromethyl-

Inchi: InChI=1S/C18H24F3NO/c1-3-5-12-22(13-6-4-2)17(23)11-10-15-8-7-9-16(14-15)18(19,20)
InchiKey: JMRJMFJETQTKT-ZHACJKMWSA-N
Formula: C18H24F3NO
SMILES: CCCCCN(CCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 327.38

Physical Properties

Property code	Value	Unit	Source
gf	-316.05	kJ/mol	Joback Method
hf	-714.70	kJ/mol	Joback Method
hfus	42.68	kJ/mol	Joback Method
hvap	63.60	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	5.147		Crippen Method
mcvol	253.280	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2078.00		NIST Webbook
tb	707.95	K	Joback Method
tc	894.34	K	Joback Method
tf	413.07	K	Joback Method
vc	0.983	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.60	J/mol×K	707.95	Joback Method
cpg	740.85	J/mol×K	739.02	Joback Method
cpg	756.14	J/mol×K	770.08	Joback Method
cpg	770.51	J/mol×K	801.15	Joback Method
cpg	784.05	J/mol×K	832.21	Joback Method
cpg	796.82	J/mol×K	863.28	Joback Method
cpg	808.89	J/mol×K	894.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308069&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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