trans-Cinnamamide, N,N-diundecyl-3-trifluoromethyl-

Inchi: InChI=1S/C32H52F3NO/c1-3-5-7-9-11-13-15-17-19-26-36(27-20-18-16-14-12-10-8-6-4-2
InchiKey: ZCVVTCJFCQUZGD-OCOZRVBESA-N
Formula: C32H52F3NO
SMILES: CCCCCCCCCCCN(CCCCCCCCCCC)C(=O)C=Cc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 523.76

Physical Properties

Property code	Value	Unit	Source
gf	-198.17	kJ/mol	Joback Method
hf	-1003.66	kJ/mol	Joback Method
hfus	78.94	kJ/mol	Joback Method
hvap	94.76	kJ/mol	Joback Method
log10ws	-11.37		Crippen Method
logp	10.609		Crippen Method
mcvol	450.540	ml/mol	McGowan Method
pc	632.25	kPa	Joback Method
tb	1028.27	K	Joback Method
tc	1276.38	K	Joback Method
tf	570.85	K	Joback Method
vc	1.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.17	J/mol×K	1028.27	Joback Method
cpg	1609.33	J/mol×K	1069.62	Joback Method
cpg	1632.25	J/mol×K	1110.97	Joback Method
cpg	1654.15	J/mol×K	1152.33	Joback Method
cpg	1675.25	J/mol×K	1193.68	Joback Method
cpg	1695.79	J/mol×K	1235.03	Joback Method
cpg	1715.99	J/mol×K	1276.38	Joback Method

Sources

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=U308079&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume