Benzamide, 2-(trifluoromethyl)-N-(2-ethylhexyl)-

Inchi: InChI=1S/C16H22F3NO/c1-3-5-8-12(4-2)11-20-15(21)13-9-6-7-10-14(13)16(17,18)19/h6

InchiKey: BHRRZMFVMXNWSZ-UHFFFAOYSA-N

Formula: C16H22F3NO

SMILES: CCCCC(CC)CNC(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 301.35

Physical Properties

Property code	Value	Unit	Source
gf	-436.94	kJ/mol	Joback Method
hf	-809.98	kJ/mol	Joback Method
hfus	35.85	kJ/mol	Joback Method
hvap	63.20	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.652		Crippen Method
mcvol	229.400	ml/mol	McGowan Method
pc	1639.10	kPa	Joback Method
rinpol	1898.00		NIST Webbook
rinpol	1898.00		NIST Webbook
tb	695.32	K	Joback Method
tc	884.23	K	Joback Method
tf	400.80	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.79	J/mol×K	695.32	Joback Method
cpg	671.38	J/mol×K	726.81	Joback Method
cpg	686.02	J/mol×K	758.29	Joback Method
cpg	699.77	J/mol×K	789.78	Joback Method
cpg	712.67	J/mol×K	821.26	Joback Method
cpg	724.78	J/mol×K	852.75	Joback Method
cpg	736.14	J/mol×K	884.23	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=U407191&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
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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