Benzamide, 2-trifluoromethyl-N-ethyl-N-2-ethylhexyl-

Inchi: InChI=1S/C18H26F3NO/c1-4-7-10-14(5-2)13-22(6-3)17(23)15-11-8-9-12-16(15)18(19,20

InchiKey: PEZCZGGOZSWARK-UHFFFAOYSA-N

Formula: C18H26F3NO

SMILES: CCCCC(CC)CN(CC)C(=O)c1ccccc1C(F)(F)F

Mol. weight [g/mol]: 329.40

Physical Properties

Property code	Value	Unit	Source
gf	-398.71	kJ/mol	Joback Method
hf	-837.20	kJ/mol	Joback Method
hfus	38.95	kJ/mol	Joback Method
hvap	63.25	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.384		Crippen Method
mcvol	257.580	ml/mol	McGowan Method
pc	1395.41	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	703.35	K	Joback Method
tc	886.88	K	Joback Method
tf	403.15	K	Joback Method
vc	0.997	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.91	J/mol×K	703.35	Joback Method
cpg	764.91	J/mol×K	733.94	Joback Method
cpg	780.91	J/mol×K	764.53	Joback Method
cpg	795.97	J/mol×K	795.12	Joback Method
cpg	810.14	J/mol×K	825.70	Joback Method
cpg	823.49	J/mol×K	856.29	Joback Method
cpg	836.05	J/mol×K	886.88	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=U415605&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