Benzamide, 2,5-di(trifluoromethyl)-N-2-ethylhexyl-

Inchi: InChI=1S/C17H21F6NO/c1-3-5-6-11(4-2)10-24-15(25)13-9-12(16(18,19)20)7-8-14(13)17

InchiKey: UGYLXJBMBNREIW-UHFFFAOYSA-N

Formula: C17H21F6NO

SMILES: CCCCC(CC)CNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 369.35

Physical Properties

Property code	Value	Unit	Source
gf	-1019.74	kJ/mol	Joback Method
hf	-1439.17	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-6.71		Crippen Method
logp	5.670		Crippen Method
mcvol	248.800	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	1752.00		NIST Webbook
rinpol	1752.00		NIST Webbook
tb	717.76	K	Joback Method
tc	896.84	K	Joback Method
tf	428.78	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.02	J/mol×K	717.76	Joback Method
cpg	750.58	J/mol×K	747.61	Joback Method
cpg	764.24	J/mol×K	777.45	Joback Method
cpg	777.07	J/mol×K	807.30	Joback Method
cpg	789.13	J/mol×K	837.15	Joback Method
cpg	800.45	J/mol×K	866.99	Joback Method
cpg	811.11	J/mol×K	896.84	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=U407923&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