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

Inchi: InChI=1S/C16H19F6NO/c1-2-3-4-5-6-9-23-14(24)12-10-11(15(17,18)19)7-8-13(12)16(20
InchiKey: VFRGMOHUGQTUTP-UHFFFAOYSA-N
Formula: C16H19F6NO
SMILES: CCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 355.32

Physical Properties

Property code	Value	Unit	Source
gf	-1025.72	kJ/mol	Joback Method
hf	-1413.25	kJ/mol	Joback Method
hfus	40.81	kJ/mol	Joback Method
hvap	60.50	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	5.424		Crippen Method
mcvol	234.710	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	695.32	K	Joback Method
tc	872.20	K	Joback Method
tf	432.51	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.89	J/mol×K	695.32	Joback Method
cpg	694.90	J/mol×K	724.80	Joback Method
cpg	708.05	J/mol×K	754.28	Joback Method
cpg	720.41	J/mol×K	783.76	Joback Method
cpg	732.01	J/mol×K	813.24	Joback Method
cpg	742.92	J/mol×K	842.72	Joback Method
cpg	753.18	J/mol×K	872.20	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=U407924&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