Benzamide, 2,3,4-trifluoro-N-butyl-N-hept-2-yl-

Inchi: InChI=1S/C18H26F3NO/c1-4-6-8-9-13(3)22(12-7-5-2)18(23)14-10-11-15(19)17(21)16(14
InchiKey: QYJHFDPCFTUVNM-UHFFFAOYSA-N
Formula: C18H26F3NO
SMILES: CCCCCC(C)N(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 329.40

Physical Properties

Property code	Value	Unit	Source
gf	-420.81	kJ/mol	Joback Method
hf	-851.39	kJ/mol	Joback Method
hfus	45.59	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.315		Crippen Method
mcvol	257.580	ml/mol	McGowan Method
pc	1345.70	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	716.54	K	Joback Method
tc	895.69	K	Joback Method
tf	425.77	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.31	J/mol×K	716.54	Joback Method
cpg	761.70	J/mol×K	746.40	Joback Method
cpg	777.23	J/mol×K	776.26	Joback Method
cpg	791.92	J/mol×K	806.12	Joback Method
cpg	805.80	J/mol×K	835.98	Joback Method
cpg	818.91	J/mol×K	865.83	Joback Method
cpg	831.28	J/mol×K	895.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U415683&Units=SI

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