Benzamide, 2,4,5-trifluoro-3-methoxy-N-decyl-

Inchi:	InChI=1S/C18H26F3NO2/c1-3-4-5-6-7-8-9-10-11-22-18(23)13-12-14(19)16(21)17(24-2)1
InchiKey:	SIBCRXJJTDIYKT-UHFFFAOYSA-N
Formula:	C18H26F3NO2
SMILES:	CCCCCCCCCCNC(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]:	345.40

Physical Properties

Property code	Value	Unit	Source
gf	-554.39	kJ/mol	Joback Method
hf	-1003.86	kJ/mol	Joback Method
hfus	51.99	kJ/mol	Joback Method
hvap	73.73	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	4.983		Crippen Method
mcvol	263.450	ml/mol	McGowan Method
pc	1321.35	kPa	Joback Method
rinpol	2342.00		NIST Webbook
rinpol	2342.00		NIST Webbook
tb	782.11	K	Joback Method
tc	966.46	K	Joback Method
tf	495.71	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.49	J/mol×K	782.11	Joback Method
cpg	807.81	J/mol×K	812.83	Joback Method
cpg	822.25	J/mol×K	843.56	Joback Method
cpg	835.85	J/mol×K	874.28	Joback Method
cpg	848.60	J/mol×K	905.01	Joback Method
cpg	860.53	J/mol×K	935.73	Joback Method
cpg	871.66	J/mol×K	966.46	Joback Method

Sources

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=U407647&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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