Benzamide, 3-chloro-2-fluoro-N-octadecyl-

Inchi: InChI=1S/C25H41ClFNO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21-28-25(29)22-1
InchiKey: PAGUVOAJXUZXIO-UHFFFAOYSA-N
Formula: C25H41ClFNO
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 426.05

Physical Properties

Property code	Value	Unit	Source
gf	6.50	kJ/mol	Joback Method
hf	-616.70	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	91.59	kJ/mol	Joback Method
log10ws	-9.95		Crippen Method
logp	8.470		Crippen Method
mcvol	364.910	ml/mol	McGowan Method
pc	905.61	kPa	Joback Method
rinpol	3240.00		NIST Webbook
rinpol	3240.00		NIST Webbook
tb	948.78	K	Joback Method
tc	1161.70	K	Joback Method
tf	556.07	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.81	J/mol×K	948.78	Joback Method
cpg	1218.05	J/mol×K	984.27	Joback Method
cpg	1235.09	J/mol×K	1019.75	Joback Method
cpg	1250.99	J/mol×K	1055.24	Joback Method
cpg	1265.84	J/mol×K	1090.73	Joback Method
cpg	1279.70	J/mol×K	1126.21	Joback Method
cpg	1292.66	J/mol×K	1161.70	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=U407834&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