3'-chloro,4'-methylcapryloanilide

Inchi: InChI=1S/C15H22ClNO/c1-3-4-5-6-7-8-15(18)17-13-10-9-12(2)14(16)11-13/h9-11H,3-8H
InchiKey: DVALOEZCMKHMOP-UHFFFAOYSA-N
Formula: C15H22ClNO
SMILES: CCCCCCCC(=O)Nc1ccc(C)c(Cl)c1
Mol. weight [g/mol]: 267.79

Physical Properties

Property code	Value	Unit	Source
gf	117.11	kJ/mol	Joback Method
hf	-214.19	kJ/mol	Joback Method
hfus	38.76	kJ/mol	Joback Method
hvap	70.15	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.947		Crippen Method
mcvol	222.240	ml/mol	McGowan Method
pc	1861.11	kPa	Joback Method
rinpol	2230.00		NIST Webbook
rinpol	2230.00		NIST Webbook
tb	720.71	K	Joback Method
tc	925.62	K	Joback Method
tf	442.78	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.05	J/mol×K	720.71	Joback Method
cpg	618.25	J/mol×K	754.86	Joback Method
cpg	632.54	J/mol×K	789.01	Joback Method
cpg	645.96	J/mol×K	823.16	Joback Method
cpg	658.53	J/mol×K	857.32	Joback Method
cpg	670.29	J/mol×K	891.47	Joback Method
cpg	681.29	J/mol×K	925.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R149121&Units=SI
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

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