Propanamide, N-(3-methylphenyl)-3-chloro-

Inchi: InChI=1S/C10H12ClNO/c1-8-3-2-4-9(7-8)12-10(13)5-6-11/h2-4,7H,5-6H2,1H3,(H,12,13)
InchiKey: XZPLSUAKDONHQY-UHFFFAOYSA-N
Formula: C10H12ClNO
SMILES: Cc1cccc(NC(=O)CCCl)c1
Mol. weight [g/mol]: 197.66

Physical Properties

Property code	Value	Unit	Source
gf	84.64	kJ/mol	Joback Method
hf	-99.52	kJ/mol	Joback Method
hfus	26.20	kJ/mol	Joback Method
hvap	58.36	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.562		Crippen Method
mcvol	151.790	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1749.00		NIST Webbook
tb	601.33	K	Joback Method
tc	821.48	K	Joback Method
tf	373.91	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.15	J/mol×K	601.33	Joback Method
cpg	361.80	J/mol×K	638.02	Joback Method
cpg	373.63	J/mol×K	674.71	Joback Method
cpg	384.66	J/mol×K	711.40	Joback Method
cpg	394.93	J/mol×K	748.10	Joback Method
cpg	404.48	J/mol×K	784.79	Joback Method
cpg	413.35	J/mol×K	821.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307226&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

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