DODECYL PHENYLCARBAMATE

Other names: Carbanilic acid, n-dodecyl ester
Inchi: InChI=1S/C19H31NO2/c1-2-3-4-5-6-7-8-9-10-14-17-22-19(21)20-18-15-12-11-13-16-18/h
InchiKey: UATVIVWPWXCCFM-UHFFFAOYSA-N
Formula: C19H31NO2
SMILES: CCCCCCCCCCCCOC(=O)Nc1ccccc1
Mol. weight [g/mol]: 305.46

Physical Properties

Property code	Value	Unit	Source
af	0.9752		Cheméo Relay (1.0)
hf	-518.57	kJ/mol	Cheméo Relay (1.0)
hfus	46.89	kJ/mol	Joback Method
hvap	109.16	kJ/mol	Cheméo Relay (1.0)
ie	8.46	eV	Cheméo Relay (1.0)
log10ws	-6.22		Cheméo Relay (1.0)
logp	6.156		Crippen Method
mcvol	272.230	ml/mol	McGowan Method
pc	1421.85	kPa	Joback Method
tb	626.83	K	Cheméo Relay (1.0)
tc	867.28	K	Cheméo Relay (1.0)
tf	332.78	K	Cheméo Relay (1.0)
vc	1.023	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	829.80	J/mol×K	787.26	Joback Method
cpg	847.10	J/mol×K	819.61	Joback Method
cpg	863.35	J/mol×K	851.97	Joback Method
cpg	878.60	J/mol×K	884.32	Joback Method
cpg	892.88	J/mol×K	916.68	Joback Method
cpg	906.22	J/mol×K	949.03	Joback Method
cpg	918.67	J/mol×K	981.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5796076&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume