

Tetradecyl 3-chlorobenzoate

Inchi:	InChI=1S/C21H33ClO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-24-21(23)19-15-14-16-20(22)
InchiKey:	WCPWDTXLJHEGKP-UHFFFAOYSA-N
Formula:	C21H33ClO2
SMILES:	CCCCCCCCCCCCCOC(=O)c1cccc(Cl)c1
Mol. weight [g/mol]:	352.94

Physical Properties

Property code	Value	Unit	Source
gf	-17.13	kJ/mol	Joback Method
hf	-512.25	kJ/mol	Joback Method
hfus	50.78	kJ/mol	Joback Method
hvap	78.82	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	7.198		Crippen Method
mvol	302.670	ml/mol	McGowan Method
pc	1181.71	kPa	Joback Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tb	825.26	K	Joback Method
tc	1021.88	K	Joback Method
tf	467.45	K	Joback Method
vc	1.177	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	916.32	J/molxK	825.26	Joback Method
cpg	933.67	J/molxK	858.03	Joback Method
cpg	949.95	J/molxK	890.80	Joback Method
cpg	965.19	J/molxK	923.57	Joback Method
cpg	979.45	J/molxK	956.34	Joback Method
cpg	992.75	J/molxK	989.11	Joback Method
cpg	1005.13	J/molxK	1021.88	Joback Method
dvisc	0.0007730	Paxs	467.45	Joback Method

dvisc	0.0003916	Paxs	527.09	Joback Method
dvisc	0.0002278	Paxs	586.72	Joback Method
dvisc	0.0001464	Paxs	646.36	Joback Method
dvisc	0.0001014	Paxs	705.99	Joback Method
dvisc	0.0000744	Paxs	765.62	Joback Method
dvisc	0.0000571	Paxs	825.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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