

Adipic acid, 2-chloro-5-methylphenyl heptyl ester

Inchi:	InChI=1S/C20H29ClO4/c1-3-4-5-6-9-14-24-19(22)10-7-8-11-20(23)25-18-15-16(2)12-13
InchiKey:	DMZIROYKJAOMTD-UHFFFAOYSA-N
Formula:	C20H29ClO4
SMILES:	CCCCCCCOC(=O)CCCCC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	368.89

Physical Properties

Property code	Value	Unit	Source
gf	-269.10	kJ/mol	Joback Method
hf	-747.88	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	86.41	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.628		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	2631.00		NIST Webbook
tb	883.65	K	Joback Method
tc	1089.89	K	Joback Method
tf	540.86	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.12	J/molxK	883.65	Joback Method
cpg	967.13	J/molxK	1055.52	Joback Method
cpg	956.77	J/molxK	1021.14	Joback Method
cpg	945.31	J/molxK	986.77	Joback Method
cpg	932.72	J/molxK	952.40	Joback Method
cpg	919.00	J/molxK	918.02	Joback Method
cpg	976.41	J/molxK	1089.89	Joback Method
dvisc	0.0000480	Paxs	883.65	Joback Method
dvisc	0.0000609	Paxs	826.52	Joback Method

dvisc	0.0000799	Paxs	769.39	Joback Method
dvisc	0.0001097	Paxs	712.25	Joback Method
dvisc	0.0001590	Paxs	655.12	Joback Method
dvisc	0.0002474	Paxs	597.99	Joback Method
dvisc	0.0004227	Paxs	540.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353962&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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