

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

Inchi:	InChI=1S/C15H19ClO4/c1-3-19-14(17)6-4-5-7-15(18)20-13-10-11(2)8-9-12(13)16/h8-10
InchiKey:	KBSHCVCALKHYFO-UHFFFAOYSA-N
Formula:	C15H19ClO4
SMILES:	CCOC(=O)CCCCC(=O)Oc1cc(C)ccc1Cl
Mol. weight [g/mol]:	298.76

Physical Properties

Property code	Value	Unit	Source
gf	-311.20	kJ/mol	Joback Method
hf	-644.68	kJ/mol	Joback Method
hfus	37.64	kJ/mol	Joback Method
hvap	75.28	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	3.677		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	769.25	K	Joback Method
tc	977.26	K	Joback Method
tf	484.51	K	Joback Method
vc	0.865	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.97	J/mol×K	769.25	Joback Method
cpg	632.56	J/mol×K	803.92	Joback Method
cpg	645.21	J/mol×K	838.59	Joback Method
cpg	656.93	J/mol×K	873.25	Joback Method
cpg	667.71	J/mol×K	907.92	Joback Method
cpg	677.58	J/mol×K	942.59	Joback Method
cpg	686.52	J/mol×K	977.26	Joback Method
dvisc	0.0006726	Paxs	484.51	Joback Method

dvisc	0.0004197	Paxs	531.97	Joback Method
dvisc	0.0002829	Paxs	579.42	Joback Method
dvisc	0.0002024	Paxs	626.88	Joback Method
dvisc	0.0001519	Paxs	674.34	Joback Method
dvisc	0.0001183	Paxs	721.79	Joback Method
dvisc	0.0000950	Paxs	769.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353956&Units=SI

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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