

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

Inchi:	InChI=1S/C17H23ClO4/c1-12(2)11-21-16(19)6-4-5-7-17(20)22-15-10-13(3)8-9-14(15)18
InchiKey:	PRIYAETYHQFLRD-UHFFFAOYSA-N
Formula:	C17H23ClO4
SMILES:	<chem>Cc1ccc(Cl)c(OC(=O)CCCC(=O)OCC(C)C)c1</chem>
Mol. weight [g/mol]:	326.81

Physical Properties

Property code	Value	Unit	Source
gf	-296.80	kJ/mol	Joback Method
hf	-691.24	kJ/mol	Joback Method
hfus	39.30	kJ/mol	Joback Method
hvap	79.34	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	4.313		Crippen Method
mcvol	253.750	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2283.00		NIST Webbook
tb	814.57	K	Joback Method
tc	1022.39	K	Joback Method
tf	492.05	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.92	J/molxK	814.57	Joback Method
cpg	792.25	J/molxK	987.76	Joback Method
cpg	782.05	J/molxK	953.12	Joback Method
cpg	770.83	J/molxK	918.48	Joback Method
cpg	758.58	J/molxK	883.84	Joback Method
cpg	745.28	J/molxK	849.21	Joback Method
cpg	801.44	J/molxK	1022.39	Joback Method
dvisc	0.0000670	Paxs	814.57	Joback Method
dvisc	0.0000853	Paxs	760.82	Joback Method

dvisc	0.0001127	Paxs	707.06	Joback Method
dvisc	0.0001559	Paxs	653.31	Joback Method
dvisc	0.0002285	Paxs	599.56	Joback Method
dvisc	0.0003612	Paxs	545.80	Joback Method
dvisc	0.0006311	Paxs	492.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353957&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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