

Sebacic acid, 4-chloro-3-methylphenyl isobutyl ester

Inchi:	InChI=1S/C21H31ClO4/c1-16(2)15-25-20(23)10-8-6-4-5-7-9-11-21(24)26-18-12-13-19(2)
InchiKey:	SMAFURAKYBDVFC-UHFFFAOYSA-N
Formula:	C21H31ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCCCCCCC(=O)OCC(C)C)ccc1Cl</chem>
Mol. weight [g/mol]:	382.92

Physical Properties

Property code	Value	Unit	Source
gf	-263.12	kJ/mol	Joback Method
hf	-773.80	kJ/mol	Joback Method
hfus	49.66	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.874		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1214.05	kPa	Joback Method
rinpola	2813.00		NIST Webbook
tb	906.09	K	Joback Method
tc	1115.27	K	Joback Method
tf	537.13	K	Joback Method
vc	1.194	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.01	J/molxK	906.09	Joback Method
cpg	979.15	J/molxK	940.95	Joback Method
cpg	993.05	J/molxK	975.82	Joback Method
cpg	1005.74	J/molxK	1010.68	Joback Method
cpg	1017.23	J/molxK	1045.55	Joback Method
cpg	1027.55	J/molxK	1080.41	Joback Method
cpg	1036.72	J/molxK	1115.27	Joback Method
dvisc	0.0004181	Paxs	537.13	Joback Method
dvisc	0.0002283	Paxs	598.62	Joback Method

dvisc	0.0001395	Paxs	660.12	Joback Method
dvisc	0.0000927	Paxs	721.61	Joback Method
dvisc	0.0000657	Paxs	783.10	Joback Method
dvisc	0.0000490	Paxs	844.60	Joback Method
dvisc	0.0000380	Paxs	906.09	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=U354844&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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