Sebacic acid, 4-chloro-2-methylbenzyl ethyl ester

Inchi: InChI=1S/C20H29ClO4/c1-3-24-19(22)10-8-6-4-5-7-9-11-20(23)25-15-17-12-13-18(21)14

InchiKey: VFWUEXSWTVQFDA-UHFFFAOYSA-N

Formula: C20H29ClO4

SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1C

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	-6.26		Crippen Method
logp	5.376		Crippen Method
mcvol	296.020	ml/mol	McGowan Method
pc	1292.07	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		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/mol×K	883.65	Joback Method
cpg	919.00	J/mol×K	918.02	Joback Method
cpg	932.72	J/mol×K	952.40	Joback Method
cpg	945.31	J/mol×K	986.77	Joback Method
cpg	956.77	J/mol×K	1021.14	Joback Method
cpg	967.13	J/mol×K	1055.52	Joback Method
cpg	976.41	J/mol×K	1089.89	Joback Method
dvisc	0.0004227	Pa×s	540.86	Joback Method

dvisc	0.0002474	Pa×s	597.99	Joback Method
dvisc	0.0001590	Pa×s	655.12	Joback Method
dvisc	0.0001097	Pa×s	712.25	Joback Method
dvisc	0.0000799	Pa×s	769.39	Joback Method
dvisc	0.0000609	Pa×s	826.52	Joback Method
dvisc	0.0000480	Pa×s	883.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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