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

Inchi: InChI=1S/C21H31ClO4/c1-3-14-25-20(23)10-8-6-4-5-7-9-11-21(24)26-16-18-12-13-19(22

InchiKey: DNMZYSYCRPBZGH-UHFFFAOYSA-N

Formula: C21H31ClO4

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

Mol. weight [g/mol]: 382.92

Physical Properties

Property code	Value	Unit	Source
gf	-260.68	kJ/mol	Joback Method
hf	-768.52	kJ/mol	Joback Method
hfus	53.18	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	5.766		Crippen Method
mcvol	310.110	ml/mol	McGowan Method
pc	1207.31	kPa	Joback Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook
tb	906.53	K	Joback Method
tc	1114.56	K	Joback Method
tf	552.13	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.52	J/mol×K	906.53	Joback Method
cpg	978.62	J/mol×K	941.20	Joback Method
cpg	992.49	J/mol×K	975.87	Joback Method
cpg	1005.17	J/mol×K	1010.55	Joback Method
cpg	1016.69	J/mol×K	1045.22	Joback Method
cpg	1027.05	J/mol×K	1079.89	Joback Method
cpg	1036.30	J/mol×K	1114.56	Joback Method
dvisc	0.0003804	Pa×s	552.13	Joback Method

dvisc	0.0002201	Pa×s	611.20	Joback Method
dvisc	0.0001402	Pa×s	670.26	Joback Method
dvisc	0.0000961	Pa×s	729.33	Joback Method
dvisc	0.0000697	Pa×s	788.40	Joback Method
dvisc	0.0000529	Pa×s	847.46	Joback Method
dvisc	0.0000416	Pa×s	906.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380585&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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