Sebacic acid, ethyl 4-methylbenzyl ester

Inchi: InChI=1S/C20H30O4/c1-3-23-19(21)10-8-6-4-5-7-9-11-20(22)24-16-18-14-12-17(2)13-15
InchiKey: TYLKCRBKTZPJCU-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CCOC(=O)CCCCCCCCC(=O)OCc1ccc(C)cc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-247.54	kJ/mol	Joback Method
hf	-720.67	kJ/mol	Joback Method
hfus	46.78	kJ/mol	Joback Method
hvap	81.36	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.722		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1341.76	kPa	Joback Method
rinpol	2481.00		NIST Webbook
rinpol	2481.00		NIST Webbook
tb	841.24	K	Joback Method
tc	1041.25	K	Joback Method
tf	498.42	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.72	J/mol×K	841.24	Joback Method
cpg	947.32	J/mol×K	1007.91	Joback Method
cpg	935.56	J/mol×K	974.58	Joback Method
cpg	922.75	J/mol×K	941.24	Joback Method
cpg	908.85	J/mol×K	907.91	Joback Method
cpg	893.85	J/mol×K	874.57	Joback Method
cpg	958.03	J/mol×K	1041.25	Joback Method
dvisc	0.0000548	Pa×s	841.24	Joback Method

dvisc	0.0000705	Pa×s	784.10	Joback Method
dvisc	0.0000945	Pa×s	726.97	Joback Method
dvisc	0.0001329	Pa×s	669.83	Joback Method
dvisc	0.0001994	Pa×s	612.69	Joback Method
dvisc	0.0003251	Pa×s	555.56	Joback Method
dvisc	0.0005930	Pa×s	498.42	Joback Method

Sources

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=U380701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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