Sebacic acid, isobutyl phenyl ester

Inchi: InChI=1S/C20H30O4/c1-17(2)16-23-19(21)14-10-5-3-4-6-11-15-20(22)24-18-12-8-7-9-13
InchiKey: KDKJNCBFFVINCP-UHFFFAOYSA-N
Formula: C20H30O4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccccc1
Mol. weight [g/mol]: 334.45

Physical Properties

Property code	Value	Unit	Source
gf	-240.35	kJ/mol	Joback Method
hf	-714.48	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	80.31	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.912		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	2512.00		NIST Webbook
rinpol	2512.00		NIST Webbook
tb	835.82	K	Joback Method
tc	1036.72	K	Joback Method
tf	470.90	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	878.85	J/mol×K	835.82	Joback Method
cpg	949.30	J/mol×K	1003.23	Joback Method
cpg	937.41	J/mol×K	969.75	Joback Method
cpg	924.45	J/mol×K	936.27	Joback Method
cpg	910.39	J/mol×K	902.79	Joback Method
cpg	895.20	J/mol×K	869.30	Joback Method
cpg	960.15	J/mol×K	1036.72	Joback Method
dvisc	0.0000497	Pa×s	835.82	Joback Method

dvisc	0.0000658	Pa×s	775.00	Joback Method
dvisc	0.0000915	Pa×s	714.18	Joback Method
dvisc	0.0001354	Pa×s	653.36	Joback Method
dvisc	0.0002169	Pa×s	592.54	Joback Method
dvisc	0.0003871	Pa×s	531.72	Joback Method
dvisc	0.0008026	Pa×s	470.90	Joback Method

Sources

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=U354506&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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