Sebacic acid, 4-bromophenyl isobutyl ester

Inchi: InChI=1S/C20H29BrO4/c1-16(2)15-24-19(22)9-7-5-3-4-6-8-10-20(23)25-18-13-11-17(21)
InchiKey: FOJSGXBBOCGGKL-UHFFFAOYSA-N
Formula: C20H29BrO4
SMILES: CC(C)COC(=O)CCCCCCCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 413.35

Physical Properties

Property code	Value	Unit	Source
gf	-235.66	kJ/mol	Joback Method
hf	-699.62	kJ/mol	Joback Method
hfus	48.54	kJ/mol	Joback Method
hvap	87.41	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.675		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1420.78	kPa	Joback Method
rinpol	2823.00		NIST Webbook
tb	906.96	K	Joback Method
tc	1119.93	K	Joback Method
tf	543.22	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.65	J/mol×K	906.96	Joback Method
cpg	933.17	J/mol×K	942.46	Joback Method
cpg	946.52	J/mol×K	977.95	Joback Method
cpg	958.72	J/mol×K	1013.45	Joback Method
cpg	969.82	J/mol×K	1048.94	Joback Method
cpg	979.85	J/mol×K	1084.44	Joback Method
cpg	988.85	J/mol×K	1119.93	Joback Method
dvisc	0.0004271	Pa×s	543.22	Joback Method
dvisc	0.0002349	Pa×s	603.84	Joback Method

dvisc	0.0001441	Pa×s	664.47	Joback Method
dvisc	0.0000959	Pa×s	725.09	Joback Method
dvisc	0.0000680	Pa×s	785.71	Joback Method
dvisc	0.0000506	Pa×s	846.34	Joback Method
dvisc	0.0000392	Pa×s	906.96	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=U354764&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