Sebacic acid, 4-bromophenyl heptyl ester

Inchi: InChI=1S/C23H35BrO4/c1-2-3-4-9-12-19-27-22(25)13-10-7-5-6-8-11-14-23(26)28-21-17-
InchiKey: ICTBAKSZSRBRMO-UHFFFAOYSA-N
Formula: C23H35BrO4
SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 455.43

Physical Properties

Property code	Value	Unit	Source
gf	-207.96	kJ/mol	Joback Method
hf	-756.26	kJ/mol	Joback Method
hfus	59.84	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.989		Crippen Method
mcvol	343.550	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	3204.00		NIST Webbook
rinpol	3204.00		NIST Webbook
tb	976.04	K	Joback Method
tc	1195.50	K	Joback Method
tf	592.03	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1098.41	J/mol×K	976.04	Joback Method
cpg	1161.43	J/mol×K	1158.93	Joback Method
cpg	1151.24	J/mol×K	1122.35	Joback Method
cpg	1139.90	J/mol×K	1085.77	Joback Method
cpg	1127.34	J/mol×K	1049.19	Joback Method
cpg	1113.53	J/mol×K	1012.62	Joback Method
cpg	1170.51	J/mol×K	1195.50	Joback Method
dvisc	0.0000271	Pa×s	976.04	Joback Method

dvisc	0.0000348	Pa×s	912.04	Joback Method
dvisc	0.0000465	Pa×s	848.04	Joback Method
dvisc	0.0000650	Pa×s	784.03	Joback Method
dvisc	0.0000964	Pa×s	720.03	Joback Method
dvisc	0.0001544	Pa×s	656.03	Joback Method
dvisc	0.0002740	Pa×s	592.03	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=U354768&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