Sebacic acid, di(4-bromophenyl) ester

Inchi: InChI=1S/C22H24Br2O4/c23-17-9-13-19(14-10-17)27-21(25)7-5-3-1-2-4-6-8-22(26)28-2
InchiKey: OAYRQYGBYPQZKJ-UHFFFAOYSA-N
Formula: C22H24Br2O4
SMILES: O=C(CCCCCCCCC(=O)Oc1ccc(Br)cc1)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 512.23

Physical Properties

Property code	Value	Unit	Source
gf	-99.28	kJ/mol	Joback Method
hf	-484.23	kJ/mol	Joback Method
hfus	56.18	kJ/mol	Joback Method
hvap	101.62	kJ/mol	Joback Method
log10ws	-8.59		Crippen Method
logp	6.843		Crippen Method
mcvol	323.200	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	3622.00		NIST Webbook
tb	1050.98	K	Joback Method
tc	1294.98	K	Joback Method
tf	679.50	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	959.58	J/mol×K	1050.98	Joback Method
cpg	970.29	J/mol×K	1091.65	Joback Method
cpg	979.83	J/mol×K	1132.31	Joback Method
cpg	988.27	J/mol×K	1172.98	Joback Method
cpg	995.69	J/mol×K	1213.65	Joback Method
cpg	1002.17	J/mol×K	1254.31	Joback Method
cpg	1007.79	J/mol×K	1294.98	Joback Method
dvisc	0.0001672	Pa×s	679.50	Joback Method
dvisc	0.0001068	Pa×s	741.41	Joback Method

dvisc	0.0000730	Pa×s	803.33	Joback Method
dvisc	0.0000527	Pa×s	865.24	Joback Method
dvisc	0.0000398	Pa×s	927.15	Joback Method
dvisc	0.0000311	Pa×s	989.07	Joback Method
dvisc	0.0000250	Pa×s	1050.98	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=U354772&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