Sebacic acid, 2-(4-bromophenoxy)ethyl pentyl ester

Inchi: InChI=1S/C23H35BrO5/c1-2-3-10-17-28-22(25)11-8-6-4-5-7-9-12-23(26)29-19-18-27-21-
InchiKey: FVNMCTQSPCTVAL-UHFFFAOYSA-N
Formula: C23H35BrO5
SMILES: CCCCCOC(=O)CCCCCCCCC(=O)OCCOc1ccc(Br)cc1
Mol. weight [g/mol]: 471.43

Physical Properties

Property code	Value	Unit	Source
gf	-312.96	kJ/mol	Joback Method
hf	-888.48	kJ/mol	Joback Method
hfus	61.02	kJ/mol	Joback Method
hvap	96.89	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	6.225		Crippen Method
mcvol	349.420	ml/mol	McGowan Method
pc	1136.73	kPa	Joback Method
rinpol	3199.00		NIST Webbook
rinpol	3199.00		NIST Webbook
tb	998.46	K	Joback Method
tc	1222.41	K	Joback Method
tf	614.26	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1126.34	J/mol×K	998.46	Joback Method
cpg	1140.65	J/mol×K	1035.78	Joback Method
cpg	1153.47	J/mol×K	1073.11	Joback Method
cpg	1164.83	J/mol×K	1110.43	Joback Method
cpg	1174.77	J/mol×K	1147.76	Joback Method
cpg	1183.32	J/mol×K	1185.08	Joback Method
cpg	1190.52	J/mol×K	1222.41	Joback Method
dvisc	0.0001901	Pa×s	614.26	Joback Method

dvisc	0.0001093	Pa×s	678.29	Joback Method
dvisc	0.0000691	Pa×s	742.33	Joback Method
dvisc	0.0000470	Pa×s	806.36	Joback Method
dvisc	0.0000339	Pa×s	870.39	Joback Method
dvisc	0.0000255	Pa×s	934.43	Joback Method
dvisc	0.0000199	Pa×s	998.46	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=U380597&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