Sebacic acid, 4-bromophenyl isohexyl ester

Inchi: InChI=1S/C22H33BrO4/c1-18(2)10-9-17-26-21(24)11-7-5-3-4-6-8-12-22(25)27-20-15-13-
InchiKey: XHEDREBGWADVTJ-UHFFFAOYSA-N
Formula: C22H33BrO4
SMILES: CC(C)CCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 441.40

Physical Properties

Property code	Value	Unit	Source
gf	-218.82	kJ/mol	Joback Method
hf	-740.90	kJ/mol	Joback Method
hfus	53.72	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.455		Crippen Method
mcvol	329.460	ml/mol	McGowan Method
pc	1235.48	kPa	Joback Method
rinpol	3061.00		NIST Webbook
tb	952.72	K	Joback Method
tc	1169.39	K	Joback Method
tf	565.76	K	Joback Method
vc	1.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.17	J/mol×K	952.72	Joback Method
cpg	1053.06	J/mol×K	988.83	Joback Method
cpg	1066.69	J/mol×K	1024.94	Joback Method
cpg	1079.08	J/mol×K	1061.05	Joback Method
cpg	1090.30	J/mol×K	1097.16	Joback Method
cpg	1100.39	J/mol×K	1133.28	Joback Method
cpg	1109.38	J/mol×K	1169.39	Joback Method
dvisc	0.0003371	Pa×s	565.76	Joback Method
dvisc	0.0001815	Pa×s	630.25	Joback Method

dvisc	0.0001096	Pa×s	694.75	Joback Method
dvisc	0.0000721	Pa×s	759.24	Joback Method
dvisc	0.0000507	Pa×s	823.73	Joback Method
dvisc	0.0000375	Pa×s	888.23	Joback Method
dvisc	0.0000289	Pa×s	952.72	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=U354767&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