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

Inchi: InChI=1S/C22H33BrO5/c1-18(2)17-28-22(25)10-8-6-4-3-5-7-9-21(24)27-16-15-26-20-13-

InchiKey: VTQINZKHABNMDI-UHFFFAOYSA-N

Formula: C22H33BrO5

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OCCOc1ccc(Br)cc1

Mol. weight [g/mol]: 457.40

Physical Properties

Property code	Value	Unit	Source
gf	-323.82	kJ/mol	Joback Method
hf	-873.12	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	94.27	kJ/mol	Joback Method
log10ws	-6.52		Crippen Method
logp	5.691		Crippen Method
mcvol	335.330	ml/mol	McGowan Method
pc	1220.85	kPa	Joback Method
rinpol	3077.00		NIST Webbook
rinpol	3077.00		NIST Webbook
tb	975.14	K	Joback Method
tc	1195.07	K	Joback Method
tf	587.99	K	Joback Method
vc	1.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1066.18	J/mol×K	975.14	Joback Method
cpg	1080.30	J/mol×K	1011.79	Joback Method
cpg	1092.99	J/mol×K	1048.45	Joback Method
cpg	1104.29	J/mol×K	1085.10	Joback Method
cpg	1114.22	J/mol×K	1121.76	Joback Method
cpg	1122.82	J/mol×K	1158.41	Joback Method
cpg	1130.11	J/mol×K	1195.07	Joback Method
dvisc	0.0002325	Pa×s	587.99	Joback Method

dvisc	0.0001281	Pa×s	652.51	Joback Method
dvisc	0.0000785	Pa×s	717.04	Joback Method
dvisc	0.0000522	Pa×s	781.56	Joback Method
dvisc	0.0000369	Pa×s	846.09	Joback Method
dvisc	0.0000275	Pa×s	910.61	Joback Method
dvisc	0.0000212	Pa×s	975.14	Joback Method

Sources

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=U380596&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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