Terephthalic acid, 2-bromophenethyl heptyl ester

Inchi: InChI=1S/C23H27BrO4/c1-2-3-4-5-8-16-27-22(25)19-11-13-20(14-12-19)23(26)28-17-15

InchiKey: ZTGKWGPSRNRWOI-UHFFFAOYSA-N

Formula: C23H27BrO4

SMILES: CCCCCCCOC(=O)c1ccc(C(=O)OCCc2ccccc2Br)cc1

Mol. weight [g/mol]: 447.36

Physical Properties

Property code	Value	Unit	Source
gf	-105.18	kJ/mol	Joback Method
hf	-531.20	kJ/mol	Joback Method
hfus	53.49	kJ/mol	Joback Method
hvap	97.42	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	5.976		Crippen Method
mcvol	319.790	ml/mol	McGowan Method
pc	1442.44	kPa	Joback Method
rinpol	2514.00		NIST Webbook
rinpol	2514.00		NIST Webbook
tb	1007.70	K	Joback Method
tc	1241.48	K	Joback Method
tf	630.97	K	Joback Method
vc	1.218	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.51	J/mol×K	1007.70	Joback Method
cpg	1001.91	J/mol×K	1046.66	Joback Method
cpg	1013.00	J/mol×K	1085.63	Joback Method
cpg	1022.83	J/mol×K	1124.59	Joback Method
cpg	1031.46	J/mol×K	1163.55	Joback Method
cpg	1038.96	J/mol×K	1202.51	Joback Method
cpg	1045.39	J/mol×K	1241.48	Joback Method
dvisc	0.0002246	Pa×s	630.97	Joback Method

dvisc	0.0001367	Pa×s	693.76	Joback Method
dvisc	0.0000903	Pa×s	756.55	Joback Method
dvisc	0.0000636	Pa×s	819.34	Joback Method
dvisc	0.0000471	Pa×s	882.12	Joback Method
dvisc	0.0000363	Pa×s	944.91	Joback Method
dvisc	0.0000289	Pa×s	1007.70	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=U416027&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