Terephthalic acid, 2-bromophenethyl butyl ester

Inchi: InChI=1S/C20H21BrO4/c1-2-3-13-24-19(22)16-8-10-17(11-9-16)20(23)25-14-12-15-6-4-5

InchiKey: OOQLCLXUOCQYGW-UHFFFAOYSA-N

Formula: C20H21BrO4

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

Mol. weight [g/mol]: 405.28

Physical Properties

Property code	Value	Unit	Source
gf	-130.44	kJ/mol	Joback Method
hf	-469.28	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.806		Crippen Method
mcvol	277.520	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	3017.00		NIST Webbook
rinpol	3017.00		NIST Webbook
tb	939.06	K	Joback Method
tc	1173.28	K	Joback Method
tf	597.16	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.72	J/mol×K	939.06	Joback Method
cpg	825.86	J/mol×K	978.10	Joback Method
cpg	836.75	J/mol×K	1017.13	Joback Method
cpg	846.44	J/mol×K	1056.17	Joback Method
cpg	854.98	J/mol×K	1095.21	Joback Method
cpg	862.41	J/mol×K	1134.24	Joback Method
cpg	868.78	J/mol×K	1173.28	Joback Method
dvisc	0.0003142	Pa×s	597.16	Joback Method

dvisc	0.0001976	Pa×s	654.14	Joback Method
dvisc	0.0001339	Pa×s	711.13	Joback Method
dvisc	0.0000961	Pa×s	768.11	Joback Method
dvisc	0.0000722	Pa×s	825.09	Joback Method
dvisc	0.0000563	Pa×s	882.08	Joback Method
dvisc	0.0000452	Pa×s	939.06	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=U416024&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