2-Bromobenzoic acid, tridec-2-ynyl ester

Inchi: InChI=1S/C20H27BrO2/c1-2-3-4-5-6-7-8-9-10-11-14-17-23-20(22)18-15-12-13-16-19(18)
InchiKey: FYEKZGXVPYTJIC-UHFFFAOYSA-N
Formula: C20H27BrO2
SMILES: CCCCCCCCCCC#CCOC(=O)c1ccccc1Br
Mol. weight [g/mol]: 379.33

Physical Properties

Property code	Value	Unit	Source
gf	203.50	kJ/mol	Joback Method
hf	-177.24	kJ/mol	Joback Method
hfus	52.40	kJ/mol	Joback Method
hvap	80.80	kJ/mol	Joback Method
log10ws	-7.69		Crippen Method
logp	6.140		Crippen Method
mcvol	285.240	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	2714.00		NIST Webbook
tb	840.11	K	Joback Method
tc	1056.05	K	Joback Method
tf	592.16	K	Joback Method
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.60	J/mol×K	840.11	Joback Method
cpg	837.65	J/mol×K	876.10	Joback Method
cpg	852.64	J/mol×K	912.09	Joback Method
cpg	866.61	J/mol×K	948.08	Joback Method
cpg	879.60	J/mol×K	984.07	Joback Method
cpg	891.67	J/mol×K	1020.06	Joback Method
cpg	902.86	J/mol×K	1056.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299400&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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