2-(Neopentyloxycarbonyl)benzoic acid

Inchi: InChI=1S/C13H16O4/c1-13(2,3)8-17-12(16)10-7-5-4-6-9(10)11(14)15/h4-7H,8H2,1-3H3,
InchiKey: FSEWDIPTRJFLRS-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: CC(C)(C)COC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 236.26
CAS: 83646-70-2

Physical Properties

Property code	Value	Unit	Source
gf	-335.46	kJ/mol	Joback Method
hf	-604.95	kJ/mol	Joback Method
hfus	24.14	kJ/mol	Joback Method
hvap	78.76	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	2.588		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1809.00		NIST Webbook
tb	747.61	K	Joback Method
tc	955.90	K	Joback Method
tf	460.54	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.46	J/mol×K	747.61	Joback Method
cpg	529.15	J/mol×K	782.33	Joback Method
cpg	540.00	J/mol×K	817.04	Joback Method
cpg	550.07	J/mol×K	851.76	Joback Method
cpg	559.39	J/mol×K	886.47	Joback Method
cpg	568.01	J/mol×K	921.19	Joback Method
cpg	575.94	J/mol×K	955.90	Joback Method

dvisc	0.0008855	Pa×s	460.54	Joback Method
dvisc	0.0003838	Pa×s	508.38	Joback Method
dvisc	0.0001921	Pa×s	556.23	Joback Method
dvisc	0.0001073	Pa×s	604.08	Joback Method
dvisc	0.0000652	Pa×s	651.92	Joback Method
dvisc	0.0000425	Pa×s	699.76	Joback Method
dvisc	0.0000292	Pa×s	747.61	Joback Method

Sources

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=C83646702&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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