2-(Heptyloxycarbonyl)benzoic acid

Inchi: InChI=1S/C15H20O4/c1-2-3-4-5-8-11-19-15(18)13-10-7-6-9-12(13)14(16)17/h6-7,9-10H,
InchiKey: DMVQNBGDYPFJCC-UHFFFAOYSA-N
Formula: C15H20O4
SMILES: CCCCCCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 264.32
CAS: 24539-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-321.46	kJ/mol	Joback Method
hf	-637.48	kJ/mol	Joback Method
hfus	36.73	kJ/mol	Joback Method
hvap	84.50	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.512		Crippen Method
mcvol	213.330	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	796.60	K	Joback Method
tc	994.81	K	Joback Method
tf	480.66	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.14	J/mol×K	796.60	Joback Method
cpg	635.53	J/mol×K	829.64	Joback Method
cpg	647.09	J/mol×K	862.67	Joback Method
cpg	657.85	J/mol×K	895.71	Joback Method
cpg	667.84	J/mol×K	928.74	Joback Method
cpg	677.07	J/mol×K	961.78	Joback Method
cpg	685.57	J/mol×K	994.81	Joback Method

dvisc	0.0007019	Pa×s	480.66	Joback Method
dvisc	0.0003062	Pa×s	533.32	Joback Method
dvisc	0.0001550	Pa×s	585.97	Joback Method
dvisc	0.0000878	Pa×s	638.63	Joback Method
dvisc	0.0000542	Pa×s	691.29	Joback Method
dvisc	0.0000359	Pa×s	743.94	Joback Method
dvisc	0.0000251	Pa×s	796.60	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=C24539580&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