2-((Octan-2-yloxy)carbonyl)benzoic acid

Other names: 2-((Octan-2-yloxy)carbonyl)benzoic acid
Inchi: InChI=1S/C16H22O4/c1-3-4-5-6-9-12(2)20-16(19)14-11-8-7-10-13(14)15(17)18/h7-8,10-
InchiKey: DUJBEEUYBSLMGM-UHFFFAOYSA-N
Formula: C16H22O4
SMILES: CCCCCCC(C)OC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
hf	-781.06	kJ/mol	Cheméo Relay (1.0)
hfus	35.80	kJ/mol	Joback Method
hvap	106.39	kJ/mol	Cheméo Relay (1.0)
ie	9.27	eV	Cheméo Relay (1.0)
log10ws	-4.10		Cheméo Relay (1.0)
logp	3.901		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2143.00		NIST Webbook
rinpol	2143.00		NIST Webbook
tb	604.93	K	Cheméo Relay (1.0)
tf	338.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.33	J/mol×K	819.04	Joback Method
cpg	692.23	J/mol×K	852.41	Joback Method
cpg	704.24	J/mol×K	885.78	Joback Method
cpg	715.38	J/mol×K	919.15	Joback Method
cpg	725.69	J/mol×K	952.52	Joback Method
cpg	735.19	J/mol×K	985.90	Joback Method
cpg	743.90	J/mol×K	1019.27	Joback Method
dvisc	0.0007462	Pa×s	476.93	Joback Method
dvisc	0.0002933	Pa×s	533.95	Joback Method

dvisc	0.0001380	Pa×s	590.97	Joback Method
dvisc	0.0000742	Pa×s	647.99	Joback Method
dvisc	0.0000441	Pa×s	705.00	Joback Method
dvisc	0.0000283	Pa×s	762.02	Joback Method
dvisc	0.0000193	Pa×s	819.04	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68296979&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tf:	Normal melting (fusion) point