2-((3,5,5-Trimethylhexyloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C17H24O4/c1-12(11-17(2,3)4)9-10-21-16(20)14-8-6-5-7-13(14)15(18)19/h5-8,

InchiKey: RJFYLVAMNLWRKY-UHFFFAOYSA-N

Formula: C17H24O4

SMILES: CC(CCOC(=O)c1ccccc1C(=O)O)CC(C)(C)C

Mol. weight [g/mol]: 292.37

CAS: 297182-83-3

Physical Properties

Property code	Value	Unit	Source
gf	-304.22	kJ/mol	Joback Method
hf	-692.79	kJ/mol	Joback Method
hfus	30.98	kJ/mol	Joback Method
hvap	87.27	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.004		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1880.53	kPa	Joback Method
rinpol	2213.00		NIST Webbook
tb	838.69	K	Joback Method
tc	1044.60	K	Joback Method
tf	490.62	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.20	J/mol×K	838.69	Joback Method
cpg	794.90	J/mol×K	1010.28	Joback Method
cpg	785.04	J/mol×K	975.96	Joback Method
cpg	774.39	J/mol×K	941.64	Joback Method
cpg	762.90	J/mol×K	907.33	Joback Method
cpg	750.52	J/mol×K	873.01	Joback Method
cpg	804.01	J/mol×K	1044.60	Joback Method
dvisc	0.0000129	Pa×s	838.69	Joback Method

dvisc	0.0000192	Pa×s	780.68	Joback Method
dvisc	0.0000306	Pa×s	722.67	Joback Method
dvisc	0.0000527	Pa×s	664.65	Joback Method
dvisc	0.0001008	Pa×s	606.64	Joback Method
dvisc	0.0002210	Pa×s	548.63	Joback Method
dvisc	0.0005837	Pa×s	490.62	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=C297182833&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