p-n-Octadecyloxybenzoic acid

Inchi: InChI=1S/C25H42O3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-22-28-24-20-18-23(19
InchiKey: TZEWVAHWYIHCEC-UHFFFAOYSA-N
Formula: C25H42O3
SMILES: CCCCCCCCCCCCCCCCCCOc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 390.60
CAS: 15872-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-108.34	kJ/mol	Joback Method
hf	-731.30	kJ/mol	Joback Method
hfus	61.03	kJ/mol	Joback Method
hvap	100.02	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	8.025		Crippen Method
mcvol	352.660	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
tb	971.53	K	Joback Method
tc	1192.15	K	Joback Method
tf	378.00 ± 1.00	K	NIST Webbook
vc	1.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.66	J/mol×K	971.53	Joback Method
cpg	1217.67	J/mol×K	1008.30	Joback Method
cpg	1234.35	J/mol×K	1045.07	Joback Method
cpg	1249.75	J/mol×K	1081.84	Joback Method
cpg	1263.94	J/mol×K	1118.61	Joback Method
cpg	1277.00	J/mol×K	1155.38	Joback Method
cpg	1289.00	J/mol×K	1192.15	Joback Method
cps	145.00	J/mol×K	320.00	NIST Webbook
dvisc	0.0002246	Pa×s	543.43	Joback Method

dvisc	0.0000817	Pa×s	614.78	Joback Method
dvisc	0.0000367	Pa×s	686.13	Joback Method
dvisc	0.0000192	Pa×s	757.48	Joback Method
dvisc	0.0000112	Pa×s	828.83	Joback Method
dvisc	0.0000071	Pa×s	900.18	Joback Method
dvisc	0.0000048	Pa×s	971.53	Joback Method

Sources

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=C15872501&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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