Benzeneacetic acid, decyl ester

Other names: phenylacetic acid decyl ester
Inchi: InChI=1S/C18H28O2/c1-2-3-4-5-6-7-8-12-15-20-18(19)16-17-13-10-9-11-14-17/h9-11,13
InchiKey: AKKHCVAUQXJEOR-UHFFFAOYSA-N
Formula: C18H28O2
SMILES: CCCCCCCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]: 276.41

Physical Properties

Property code	Value	Unit	Source
gf	-20.83	kJ/mol	Joback Method
hf	-423.12	kJ/mol	Joback Method
hfus	39.20	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.913		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2005.97		NIST Webbook
rinpol	2005.97		NIST Webbook
rinpol	2035.66		NIST Webbook
tb	714.21	K	Joback Method
tc	906.19	K	Joback Method
tf	391.20	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.91	J/mol×K	714.21	Joback Method
cpg	728.69	J/mol×K	746.21	Joback Method
cpg	745.47	J/mol×K	778.20	Joback Method
cpg	761.28	J/mol×K	810.20	Joback Method
cpg	776.16	J/mol×K	842.20	Joback Method
cpg	790.14	J/mol×K	874.20	Joback Method

cpg	803.25	J/mol×K	906.19	Joback Method
dvisc	0.0015490	Pa×s	391.20	Joback Method
dvisc	0.0007359	Pa×s	445.03	Joback Method
dvisc	0.0004105	Pa×s	498.87	Joback Method
dvisc	0.0002566	Pa×s	552.70	Joback Method
dvisc	0.0001743	Pa×s	606.54	Joback Method
dvisc	0.0001261	Pa×s	660.38	Joback Method
dvisc	0.0000958	Pa×s	714.21	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=U281803&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

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