Benzeneacetic acid, heptyl ester

Other names:	Heptyl phenylacetate
	Phenylacetic acid heptyl ester
	NSC 406420
Inchi:	InChI=1S/C15H22O2/c1-2-3-4-5-9-12-17-15(16)13-14-10-7-6-8-11-14/h6-8,10-11H,2-5,9
InchiKey:	MFCMCQJYPOAXCB-UHFFFAOYSA-N
Formula:	C15H22O2
SMILES:	CCCCCCCOC(=O)Cc1ccccc1
Mol. weight [g/mol]:	234.33
CAS:	39736-25-9

Physical Properties

Property code	Value	Unit	Source
gf	-46.09	kJ/mol	Joback Method
hf	-361.20	kJ/mol	Joback Method
hfus	31.43	kJ/mol	Joback Method
hvap	60.42	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.743		Crippen Method
mcvol	205.890	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	1707.67		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1733.01		NIST Webbook
ripol	2265.00		NIST Webbook
ripol	2266.00		NIST Webbook
ripol	2266.00		NIST Webbook
tb	645.57	K	Joback Method
tc	843.08	K	Joback Method
tf	357.39	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.39	J/mol×K	645.57	Joback Method
cpg	563.17	J/mol×K	678.49	Joback Method
cpg	579.02	J/mol×K	711.41	Joback Method
cpg	593.96	J/mol×K	744.32	Joback Method
cpg	608.02	J/mol×K	777.24	Joback Method
cpg	621.23	J/mol×K	810.16	Joback Method
cpg	633.62	J/mol×K	843.08	Joback Method
dvisc	0.0019370	Pa×s	357.39	Joback Method
dvisc	0.0009578	Pa×s	405.42	Joback Method
dvisc	0.0005498	Pa×s	453.45	Joback Method
dvisc	0.0003510	Pa×s	501.48	Joback Method
dvisc	0.0002424	Pa×s	549.51	Joback Method
dvisc	0.0001776	Pa×s	597.54	Joback Method
dvisc	0.0001364	Pa×s	645.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39736259&Units=SI
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

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
ripol: Polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume