

2-phenylethyl levulinate

Inchi:	InChI=1S/C13H16O3/c1-11(14)7-8-13(15)16-10-9-12-5-3-2-4-6-12/h2-6H,7-10H2,1H3
InchiKey:	FJEDCBJSNFURKI-UHFFFAOYSA-N
Formula:	C13H16O3
SMILES:	CC(=O)CCC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	220.26

Physical Properties

Property code	Value	Unit	Source
gf	-191.85	kJ/mol	Joback Method
hf	-432.50	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	62.71	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	2.141		Crippen Method
mvol	179.280	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
ripol	2617.00		NIST Webbook
ripol	2617.00		NIST Webbook
tb	653.68	K	Joback Method
tc	863.60	K	Joback Method
tf	384.78	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	462.59	J/molxK	653.68	Joback Method
cpg	476.96	J/molxK	688.67	Joback Method
cpg	490.43	J/molxK	723.65	Joback Method
cpg	503.02	J/molxK	758.64	Joback Method
cpg	514.76	J/molxK	793.62	Joback Method
cpg	525.67	J/molxK	828.61	Joback Method
cpg	535.78	J/molxK	863.60	Joback Method
dvisc	0.0017744	Paxs	384.78	Joback Method

dvisc	0.0009819	Paxs	429.60	Joback Method
dvisc	0.0006076	Paxs	474.41	Joback Method
dvisc	0.0004085	Paxs	519.23	Joback Method
dvisc	0.0002925	Paxs	564.05	Joback Method
dvisc	0.0002200	Paxs	608.86	Joback Method
dvisc	0.0001721	Paxs	653.68	Joback Method

Sources

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=R321398&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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