

Butyric acid, 2-phenyl-, cyclohexylmethyl ester

Inchi:	InChI=1S/C17H24O2/c1-2-16(15-11-7-4-8-12-15)17(18)19-13-14-9-5-3-6-10-14/h4,7-8,1
InchiKey:	QGVVFERCLIIXMH-UHFFFAOYSA-N
Formula:	C17H24O2
SMILES:	CCC(C(=O)OCC1CCCCC1)c1ccccc1
Mol. weight [g/mol]:	260.37

Physical Properties

Property code	Value	Unit	Source
gf	-7.24	kJ/mol	Joback Method
hf	-353.44	kJ/mol	Joback Method
hfus	24.93	kJ/mol	Joback Method
hvap	64.91	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.304		Crippen Method
mvol	223.210	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1900.00		NIST Webbook
tb	710.44	K	Joback Method
tc	936.90	K	Joback Method
tf	372.31	K	Joback Method
vc	0.831	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.77	J/molxK	710.44	Joback Method
cpg	670.21	J/molxK	748.18	Joback Method
cpg	689.17	J/molxK	785.93	Joback Method
cpg	706.68	J/molxK	823.67	Joback Method
cpg	722.81	J/molxK	861.41	Joback Method
cpg	737.60	J/molxK	899.15	Joback Method
cpg	751.11	J/molxK	936.90	Joback Method
dvisc	0.0024904	Paxs	372.31	Joback Method

dvisc	0.0010393	Paxs	428.66	Joback Method
dvisc	0.0005313	Paxs	485.02	Joback Method
dvisc	0.0003124	Paxs	541.38	Joback Method
dvisc	0.0002030	Paxs	597.73	Joback Method
dvisc	0.0001421	Paxs	654.09	Joback Method
dvisc	0.0001052	Paxs	710.44	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=U406861&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
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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