Butyric acid, 2-phenyl-, naphth-2-ylmethyl ester

Inchi: InChI=1S/C21H20O2/c1-2-20(18-9-4-3-5-10-18)21(22)23-15-16-12-13-17-8-6-7-11-19(17

InchiKey: REMBVPSKNNWYIO-UHFFFAOYSA-N

Formula: C21H20O2

SMILES: CCC(C(=O)OCc1ccc2ccccc2c1)c1ccccc1

Mol. weight [g/mol]: 304.38

Physical Properties

Property code	Value	Unit	Source
gf	211.42	kJ/mol	Joback Method
hf	-74.19	kJ/mol	Joback Method
hfus	34.12	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	5.077		Crippen Method
mcvol	247.210	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2527.00		NIST Webbook
rinpol	2527.00		NIST Webbook
tb	833.05	K	Joback Method
tc	1074.53	K	Joback Method
tf	481.65	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.60	J/mol×K	833.05	Joback Method
cpg	738.27	J/mol×K	873.30	Joback Method
cpg	752.68	J/mol×K	913.54	Joback Method
cpg	765.95	J/mol×K	953.79	Joback Method
cpg	778.19	J/mol×K	994.03	Joback Method
cpg	789.51	J/mol×K	1034.28	Joback Method
cpg	800.01	J/mol×K	1074.53	Joback Method
dvisc	0.0009897	Pa×s	481.65	Joback Method

dvisc	0.0005751	Pa×s	540.22	Joback Method
dvisc	0.0003716	Pa×s	598.78	Joback Method
dvisc	0.0002596	Pa×s	657.35	Joback Method
dvisc	0.0001923	Pa×s	715.92	Joback Method
dvisc	0.0001490	Pa×s	774.48	Joback Method
dvisc	0.0001197	Pa×s	833.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406869&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume