

Butyric acid, 2-phenyl-, tetradecyl ester

Inchi:	InChI=1S/C24H40O2/c1-3-5-6-7-8-9-10-11-12-13-14-18-21-26-24(25)23(4-2)22-19-16-15
InchiKey:	DAAHAXOYZWOCOL-UHFFFAOYSA-N
Formula:	C24H40O2
SMILES:	CCCCCCCCCCCCCOC(=O)C(CC)c1ccccc1
Mol. weight [g/mol]:	360.57

Physical Properties

Property code	Value	Unit	Source
gf	27.25	kJ/mol	Joback Method
hf	-552.24	kJ/mol	Joback Method
hfus	51.22	kJ/mol	Joback Method
hvap	80.06	kJ/mol	Joback Method
log10ws	-7.80		Crippen Method
logp	7.425		Crippen Method
mvol	332.700	ml/mol	McGowan Method
pc	1016.18	kPa	Joback Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook
tb	851.05	K	Joback Method
tc	1047.04	K	Joback Method
tf	443.82	K	Joback Method
vc	1.290	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1068.10	J/molxK	851.05	Joback Method
cpg	1087.47	J/molxK	883.72	Joback Method
cpg	1105.65	J/molxK	916.38	Joback Method
cpg	1122.67	J/molxK	949.05	Joback Method
cpg	1138.59	J/molxK	981.71	Joback Method
cpg	1153.46	J/molxK	1014.38	Joback Method
cpg	1167.33	J/molxK	1047.04	Joback Method
dvisc	0.0010041	Paxs	443.82	Joback Method

dvisc	0.0004084	Paxs	511.69	Joback Method
dvisc	0.0002051	Paxs	579.56	Joback Method
dvisc	0.0001190	Paxs	647.43	Joback Method
dvisc	0.0000765	Paxs	715.31	Joback Method
dvisc	0.0000532	Paxs	783.18	Joback Method
dvisc	0.0000391	Paxs	851.05	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U406025&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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