Butamirate Citrate

Other names: diethyl[2-[2-(2-phenylbutyroyloxy)ethoxy]ethyl]ammonium dihydrogen citrate
Inchi: InChI=1S/C18H29NO3/c1-4-17(16-10-8-7-9-11-16)18(20)22-15-14-21-13-12-19(5-2)6-3/h
InchiKey: DDVUMDPCZWBYRA-UHFFFAOYSA-N
Formula: C18H29NO3
SMILES: CCC(C(=O)OCCOCCN(CC)CC)c1ccccc1
Mol. weight [g/mol]: 307.43
CAS: 18109-81-4

Physical Properties

Property code	Value	Unit	Source
gf	-17.49	kJ/mol	Joback Method
hf	-493.09	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-2.94		Crippen Method
logp	3.082		Crippen Method
mcvol	264.010	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2021.00		NIST Webbook
tb	748.63	K	Joback Method
tc	941.68	K	Joback Method
tf	430.90	K	Joback Method
vc	0.990	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.81	J/mol×K	748.63	Joback Method
cpg	800.50	J/mol×K	780.81	Joback Method
cpg	817.13	J/mol×K	812.98	Joback Method
cpg	832.71	J/mol×K	845.16	Joback Method
cpg	847.27	J/mol×K	877.33	Joback Method
cpg	860.85	J/mol×K	909.51	Joback Method
cpg	873.48	J/mol×K	941.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18109814&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
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