Sarcosine, n-(2-bromobenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C24H38BrNO3/c1-3-4-5-6-7-8-9-10-11-12-13-16-19-29-23(27)20-26(2)24(28)2
InchiKey: IZNDKTAEMSJHHD-UHFFFAOYSA-N
Formula: C24H38BrNO3
SMILES: CCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1Br
Mol. weight [g/mol]: 468.48

Physical Properties

Property code	Value	Unit	Source
hf	-700.47	kJ/mol	Cheméo Relay (1.0)
hfus	64.26	kJ/mol	Joback Method
hvap	125.79	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.99		Cheméo Relay (1.0)
logp	6.765		Crippen Method
mcvol	361.750	ml/mol	McGowan Method
pc	1089.22	kPa	Joback Method
tb	693.62	K	Cheméo Relay (1.0)
tf	328.59	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.59	J/mol×K	988.94	Joback Method
cpg	1190.84	J/mol×K	1025.91	Joback Method
cpg	1205.88	J/mol×K	1062.89	Joback Method
cpg	1219.81	J/mol×K	1099.86	Joback Method
cpg	1232.70	J/mol×K	1136.83	Joback Method
cpg	1244.64	J/mol×K	1173.81	Joback Method
cpg	1255.70	J/mol×K	1210.78	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321460&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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