

Oxeladin

Other names:	Benzeneacetic acid, «alpha»,«alpha»-diethyl-, 2-[2-(diethylamino)ethoxy]ethyl ester Butyric acid, 2-ethyl-2-phenyl-, 2-(2-(diethylamino)ethoxy)ethyl ester 2-(2-Diethylaminoethoxy)ethyl «alpha»,«alpha»-diethylphenylacetate 2-(2-Diethylaminoethoxy)ethyl 2-ethyl-2-phenylbutyrate «alpha»,«alpha»-Diethylbenzeneacetic acid 2-(2-(diethylamino)ethoxy)ethyl ester Ethanol, 2-(2-(diethylamino)ethoxy)-, 2-ethyl-2-phenylbutyrate 2-Ethyl-2-phenylbutyric acid 2-(2-diethylaminoethoxy)ethyl ester
Inchi:	InChI=1S/C20H33NO3/c1-5-20(6-2,18-12-10-9-11-13-18)19(22)24-17-16-23-15-14-21(7-
InchiKey:	IQADUMSPOQKAAO-UHFFFAOYSA-N
Formula:	C20H33NO3
SMILES:	CCN(CC)CCOCCOC(=O)C(CC)(CC)c1ccccc1
Mol. weight [g/mol]:	335.48
CAS:	468-61-1

Physical Properties

Property code	Value	Unit	Source
gf	4.63	kJ/mol	Joback Method
hf	-537.84	kJ/mol	Joback Method
hfus	41.18	kJ/mol	Joback Method
hvap	74.70	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.646		Crippen Method
mcvol	292.190	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
tb	791.60	K	Joback Method
tc	987.86	K	Joback Method
tf	470.86	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.81	J/mol×K	791.60	Joback Method
cpg	918.98	J/mol×K	824.31	Joback Method

cpg	936.00	J/mol×K	857.02	Joback Method
cpg	951.92	J/mol×K	889.73	Joback Method
cpg	966.78	J/mol×K	922.44	Joback Method
cpg	980.65	J/mol×K	955.15	Joback Method
cpg	993.57	J/mol×K	987.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C468611&Units=SI

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
hvp:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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