Carbonic acid, monoamide, N-(2-ethylhexyl)-, octyl ester

Inchi: InChI=1S/C17H35NO2/c1-4-7-9-10-11-12-14-20-17(19)18-15-16(6-3)13-8-5-2/h16H,4-15

InchiKey: SDTSBTXASHYMDS-UHFFFAOYSA-N

Formula: C17H35NO2

SMILES: CCCCCCCCOC(=O)NCC(CC)CCCC

Mol. weight [g/mol]: 285.47

Physical Properties

Property code	Value	Unit	Source
gf	-54.71	kJ/mol	Joback Method
hf	-590.82	kJ/mol	Joback Method
hfus	44.15	kJ/mol	Joback Method
hvap	68.64	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	5.290		Crippen Method
mcvol	267.810	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	714.38	K	Joback Method
tc	888.42	K	Joback Method
tf	391.17	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	797.36	J/mol×K	714.38	Joback Method
cpg	815.60	J/mol×K	743.39	Joback Method
cpg	832.96	J/mol×K	772.39	Joback Method
cpg	849.48	J/mol×K	801.40	Joback Method
cpg	865.17	J/mol×K	830.40	Joback Method
cpg	880.04	J/mol×K	859.41	Joback Method
cpg	894.13	J/mol×K	888.42	Joback Method

Sources

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=U406622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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