

Carbonic acid, 2-ethylhexyl octyl ester

Inchi: InChI=1S/C17H34O3/c1-4-7-9-10-11-12-14-19-17(18)20-15-16(6-3)13-8-5-2/h16H,4-15H
InchiKey: YUDZKMQNKQWAQH-UHFFFAOYSA-N
Formula: C17H34O3
SMILES: CCCCCCOC(=O)OCC(CC)CCCC
Mol. weight [g/mol]: 286.45

Physical Properties

Property code	Value	Unit	Source
gf	-249.10	kJ/mol	Joback Method
hf	-776.51	kJ/mol	Joback Method
hfus	40.24	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-5.62		Crippen Method
logp	5.716		Crippen Method
mvol	263.700	ml/mol	McGowan Method
pc	1263.75	kPa	Joback Method
rinpol	1857.00		NIST Webbook
rinpol	1857.00		NIST Webbook
tb	686.63	K	Joback Method
tc	857.13	K	Joback Method
tf	360.74	K	Joback Method
vc	1.024	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.19	J/molxK	686.63	Joback Method
cpg	847.90	J/molxK	828.71	Joback Method
cpg	832.77	J/molxK	800.30	Joback Method
cpg	816.83	J/molxK	771.88	Joback Method
cpg	800.10	J/molxK	743.46	Joback Method
cpg	782.55	J/molxK	715.05	Joback Method
cpg	862.26	J/molxK	857.13	Joback Method
dvisc	0.0000770	Paxs	686.63	Joback Method

dvisc	0.0001045	Paxs	632.32	Joback Method
dvisc	0.0001501	Paxs	578.00	Joback Method
dvisc	0.0002326	Paxs	523.68	Joback Method
dvisc	0.0003987	Paxs	469.37	Joback Method
dvisc	0.0007870	Paxs	415.06	Joback Method
dvisc	0.0019068	Paxs	360.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U383135&Units=SI
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

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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