Octanoic acid, 2-butyl-

Other names:	2-Butyloctanoic acid
	2-Butyloctansaeure
	5-Undecanecarboxylic acid
Inchi:	InChI=1S/C12H24O2/c1-3-5-7-8-10-11(12(13)14)9-6-4-2/h11H,3-10H2,1-2H3,(H,13,14)
InchiKey:	OARDBPIZDHVTCK-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCC(CCCC)C(=O)O
Mol. weight [g/mol]:	200.32
CAS:	27610-92-0

Physical Properties

Property code	Value	Unit	Source
gf	-218.02	kJ/mol	Joback Method
hf	-561.10	kJ/mol	Joback Method
hfus	29.00	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.848		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
tb	619.57	K	Joback Method
tc	787.94	K	Joback Method
tf	320.75	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.20	J/mol×K	619.57	Joback Method
cpg	517.19	J/mol×K	647.63	Joback Method
cpg	530.57	J/mol×K	675.69	Joback Method
cpg	543.36	J/mol×K	703.75	Joback Method
cpg	555.57	J/mol×K	731.81	Joback Method
cpg	567.23	J/mol×K	759.87	Joback Method

cpg	578.34	J/mol×K	787.94	Joback Method
dvisc	0.0120962	Pa×s	320.75	Joback Method
dvisc	0.0028570	Pa×s	370.55	Joback Method
dvisc	0.0009499	Pa×s	420.36	Joback Method
dvisc	0.0003988	Pa×s	470.16	Joback Method
dvisc	0.0001977	Pa×s	519.96	Joback Method
dvisc	0.0001108	Pa×s	569.77	Joback Method
dvisc	0.0000682	Pa×s	619.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18405e+01
Coeff. B	-3.50624e+03
Coeff. C	-8.10260e+01
Temperature range (K), min.	335.12
Temperature range (K), max.	618.05

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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=C27610920&Units=SI

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume