Butanoic acid, 2-ethyl-, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester

Other names: Butyric acid, 2-ethyl-, diester with triethylene glycol
Flexol plasticizer 3GH
Plasticizer 3GH
Triethylene glycol bis(2-ethyl butyrate)
Triethylene glycol di(2-ethyl butyrate)
2-Ethylbutyric acid, diester with triethylene glycol
2-Ethylbutyric acid, triethylene glycol diester
2,2'-(Ethylenedioxy)di(ethyl 2-ethylbutyrate)
Butanoic acid, 2-ethyl-, 1,1'-[1,2-ethanediylbis(oxy-2,1-ethanediyl)] ester
NSC 406329
2,2'-ethylenedioxydiethyl bis(2-ethylbutyrate)

Inchi: InChI=1S/C18H34O6/c1-5-15(6-2)17(19)23-13-11-21-9-10-22-12-14-24-18(20)16(7-3)8-4

InchiKey: JEYLQCXBYFQJRO-UHFFFAOYSA-N

Formula: C18H34O6

SMILES: CCC(CC)C(=O)OCCOCCOCCOC(=O)C(CC)CC

Mol. weight [g/mol]: 346.46

CAS: 95-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-582.04	kJ/mol	Joback Method
hf	-1179.45	kJ/mol	Joback Method
hfus	43.28	kJ/mol	Joback Method
hvap	78.02	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.978		Crippen Method
mcvol	291.100	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
tb	807.78	K	Joback Method
tc	993.49	K	Joback Method
tf	451.40	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	912.35	J/mol×K	807.78	Joback Method
cpg	929.50	J/mol×K	838.73	Joback Method
cpg	945.56	J/mol×K	869.68	Joback Method
cpg	960.52	J/mol×K	900.64	Joback Method
cpg	974.39	J/mol×K	931.59	Joback Method
cpg	987.14	J/mol×K	962.54	Joback Method
cpg	998.78	J/mol×K	993.49	Joback Method
dvisc	0.0006705	Pa×s	451.40	Joback Method
dvisc	0.0003047	Pa×s	510.80	Joback Method
dvisc	0.0001632	Pa×s	570.19	Joback Method
dvisc	0.0000983	Pa×s	629.59	Joback Method
dvisc	0.0000647	Pa×s	688.99	Joback Method
dvisc	0.0000454	Pa×s	748.38	Joback Method
dvisc	0.0000336	Pa×s	807.78	Joback Method
hvapt	91.70	kJ/mol	420.50	NIST Webbook

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=C95089&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
hvapt: Enthalpy of vaporization at a given temperature

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