Decanedioic acid, bis(2-butoxyethyl) ester

Other names:	Dibutyoxyethyl sebacate
	Decanedioic acid, di-(2-butoxyethyl) ester
	di(Butoxyethyl) sebacate
	bis(2-butoxyethyl) sebacate
	bis(2-butoxyethyl) sebacoate
Inchi:	InChI=1S/C22H42O6/c1-3-5-15-25-17-19-27-21(23)13-11-9-7-8-10-12-14-22(24)28-20-1
InchiKey:	KZBSIGKPGIZQJQ-UHFFFAOYSA-N
Formula:	C22H42O6
SMILES:	CCCCOCCOC(=O)CCCCCCCCC(=O)OCCOCCCC
Mol. weight [g/mol]:	402.57
CAS:	141-19-5

Physical Properties

Property code	Value	Unit	Source
gf	-543.48	kJ/mol	Joback Method
hf	-1251.45	kJ/mol	Joback Method
hfus	60.69	kJ/mol	Joback Method
hvap	87.70	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.827		Crippen Method
mcvol	347.460	ml/mol	McGowan Method
pc	934.06	kPa	Joback Method
rinpol	2700.00		NIST Webbook
rinpol	2700.00		NIST Webbook
rinpol	2700.00		NIST Webbook
tb	900.18	K	Joback Method
tc	1103.22	K	Joback Method
tf	526.48	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1245.04	J/mol×K	1103.22	Joback Method

cpg	1233.89	J/mol×K	1069.38	Joback Method
cpg	1221.25	J/mol×K	1035.54	Joback Method
cpg	1207.12	J/mol×K	1001.70	Joback Method
cpg	1191.49	J/mol×K	967.86	Joback Method
cpg	1174.38	J/mol×K	934.02	Joback Method
cpg	1155.76	J/mol×K	900.18	Joback Method
dvisc	0.0003094	Pa×s	526.48	Joback Method
dvisc	0.0000218	Pa×s	900.18	Joback Method
dvisc	0.0000288	Pa×s	837.90	Joback Method
dvisc	0.0000398	Pa×s	775.61	Joback Method
dvisc	0.0000581	Pa×s	713.33	Joback Method
dvisc	0.0000911	Pa×s	651.05	Joback Method
dvisc	0.0001574	Pa×s	588.76	Joback Method
hvapt	120.30	kJ/mol	395.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141195&Units=SI
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

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

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