Diethyl azelate

Inchi: InChI=1S/C13H24O4/c1-3-16-12(14)10-8-6-5-7-9-11-13(15)17-4-2/h3-11H2,1-2H3
InchiKey: CQMYCPZZIPXILQ-UHFFFAOYSA-N
Formula: C13H24O4
SMILES: CCOC(=O)CCCCCCCC(=O)OCC
Mol. weight [g/mol]: 244.33
CAS: 624-17-9

Physical Properties

Property code	Value	Unit	Source
gf	-409.26	kJ/mol	Joback Method
hf	-801.25	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	62.84	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.843		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	1688.10		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1688.10		NIST Webbook
tb	649.42	K	Joback Method
tc	825.90	K	Joback Method
tf	380.59	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.37	J/mol×K	649.42	Joback Method
cpg	637.24	J/mol×K	796.48	Joback Method
cpg	624.81	J/mol×K	767.07	Joback Method
cpg	611.72	J/mol×K	737.66	Joback Method
cpg	597.94	J/mol×K	708.25	Joback Method

cpg	583.50	J/mol×K	678.83	Joback Method
cpg	649.00	J/mol×K	825.90	Joback Method
dvisc	0.0001354	Pa×s	649.42	Joback Method
dvisc	0.0001754	Pa×s	604.62	Joback Method
dvisc	0.0002370	Pa×s	559.81	Joback Method
dvisc	0.0003373	Pa×s	515.00	Joback Method
dvisc	0.0005134	Pa×s	470.20	Joback Method
dvisc	0.0008539	Pa×s	425.40	Joback Method
dvisc	0.0016009	Pa×s	380.59	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	445.20	K	2.40	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=C624179&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

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume