Adipic acid, butyl trans-hex-3-enyl ester

Inchi: InChI=1S/C16H28O4/c1-3-5-7-10-14-20-16(18)12-9-8-11-15(17)19-13-6-4-2/h5,7H,3-4,6
InchiKey: FLGBBJGLHAFCQK-FNORWQNLSA-N
Formula: C16H28O4
SMILES: CCC=CCCOC(=O)CCCCC(=O)OCCCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	-303.78	kJ/mol	Joback Method
hf	-745.95	kJ/mol	Joback Method
hfus	42.97	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.790		Crippen Method
mcvol	246.880	ml/mol	McGowan Method
pc	1467.98	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	722.22	K	Joback Method
tc	902.85	K	Joback Method
tf	409.32	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.41	J/mol×K	722.22	Joback Method
cpg	726.47	J/mol×K	752.33	Joback Method
cpg	741.71	J/mol×K	782.43	Joback Method
cpg	756.16	J/mol×K	812.54	Joback Method
cpg	769.83	J/mol×K	842.64	Joback Method
cpg	782.74	J/mol×K	872.75	Joback Method
cpg	794.90	J/mol×K	902.85	Joback Method
dvisc	0.0011649	Pa×s	409.32	Joback Method

dvisc	0.0005794	Pa×s	461.47	Joback Method
dvisc	0.0003321	Pa×s	513.62	Joback Method
dvisc	0.0002109	Pa×s	565.77	Joback Method
dvisc	0.0001446	Pa×s	617.92	Joback Method
dvisc	0.0001051	Pa×s	670.07	Joback Method
dvisc	0.0000801	Pa×s	722.22	Joback Method

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=U354008&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume