Hexadecanoic acid, 1,4-butanediyl ester

Other names: Palmitic acid, tetramethylene ester
1,4-Butanediol dipalmitate
Di-O-palmitoylbutane-1,4-diol
Inchi: InChI=1S/C36H70O4/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-31-35(37)39-33-29-30-34-
InchiKey: UXPYIAWFQKSHNV-UHFFFAOYSA-N
Formula: C36H70O4
SMILES: CCCCCCCCCCCCCCCC(=O)OCCCCOC(=O)CCCCCCCCCCCCCCC
Mol. weight [g/mol]: 566.94
CAS: 26719-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-215.60	kJ/mol	Joback Method
hf	-1275.97	kJ/mol	Joback Method
hfus	94.57	kJ/mol	Joback Method
hvap	114.04	kJ/mol	Joback Method
log10ws	-12.62		Crippen Method
logp	11.816		Crippen Method
mcvol	532.980	ml/mol	McGowan Method
pc	476.31	kPa	Joback Method
tb	1175.66	K	Joback Method
tc	1569.32	K	Joback Method
tf	639.80	K	Joback Method
vc	2.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2116.07	J/mol×K	1569.32	Joback Method
cpg	2001.75	J/mol×K	1175.66	Joback Method
cpg	2032.02	J/mol×K	1241.27	Joback Method
cpg	2057.15	J/mol×K	1306.88	Joback Method
cpg	2077.63	J/mol×K	1372.49	Joback Method
cpg	2093.95	J/mol×K	1438.10	Joback Method

cpg	2106.60	J/mol×K	1503.71	Joback Method
dvisc	0.0000043	Pa×s	1175.66	Joback Method
dvisc	0.0001005	Pa×s	639.80	Joback Method
dvisc	0.0000430	Pa×s	729.11	Joback Method
dvisc	0.0000221	Pa×s	818.42	Joback Method
dvisc	0.0000130	Pa×s	907.73	Joback Method
dvisc	0.0000084	Pa×s	997.04	Joback Method
dvisc	0.0000058	Pa×s	1086.35	Joback Method
hfust	162.40	kJ/mol	339.00	NIST Webbook

Sources

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=C26719631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume