Terephthalic acid, but-3-enyl heptadecyl ester

Inchi: InChI=1S/C29H46O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-25-33-29(31)27-22-2
InchiKey: FBLDAZGXKJLTHO-UHFFFAOYSA-N
Formula: C29H46O4
SMILES: C=CCCOC(=O)c1ccc(C(=O)OCCCCCCCCCCCCCCCCCC)cc1
Mol. weight [g/mol]: 458.67

Physical Properties

Property code	Value	Unit	Source
gf	-83.92	kJ/mol	Joback Method
hf	-781.00	kJ/mol	Joback Method
hfus	68.81	kJ/mol	Joback Method
hvap	100.73	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	8.448		Crippen Method
mcvol	406.290	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
rinpol	3501.00		NIST Webbook
rinpol	3501.00		NIST Webbook
tb	1043.84	K	Joback Method
tc	1285.02	K	Joback Method
tf	598.09	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.41	J/mol×K	1043.84	Joback Method
cpg	1476.43	J/mol×K	1244.82	Joback Method
cpg	1464.85	J/mol×K	1204.62	Joback Method
cpg	1451.74	J/mol×K	1164.43	Joback Method
cpg	1437.03	J/mol×K	1124.23	Joback Method
cpg	1420.61	J/mol×K	1084.04	Joback Method
cpg	1486.58	J/mol×K	1285.02	Joback Method
dvisc	0.0000155	Pa×s	1043.84	Joback Method

dvisc	0.0000204	Pa×s	969.55	Joback Method
dvisc	0.0000280	Pa×s	895.26	Joback Method
dvisc	0.0000406	Pa×s	820.97	Joback Method
dvisc	0.0000636	Pa×s	746.67	Joback Method
dvisc	0.0001098	Pa×s	672.38	Joback Method
dvisc	0.0002173	Pa×s	598.09	Joback Method

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=U356347&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
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