thiobis(ethane-2,1-diyl) bis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propanoa

Inchi: InChI=1S/C38H58O6S/c1-35(2,3)27-21-25(22-28(33(27)41)36(4,5)6)13-15-31(39)43-17-

InchiKey: VFBJXXJYHWLXRM-UHFFFAOYSA-N

Formula: C38H58O6S

SMILES: CC(C)(C)c1cc(CCC(=O)OCCSCCOC(=O)CCc2cc(C(C)(C)C)c(O)c(C(C)(C)C)c2)cc(C(C)

Mol. weight [g/mol]: 642.94

Physical Properties

Property code	Value	Unit	Source
hfus	72.32	kJ/mol	Joback Method
logp	8.673		Crippen Method
mcvol	541.730	ml/mol	McGowan Method
tf	387.92	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2211.74	J/mol×K	1511.80	Joback Method
cpg	2284.67	J/mol×K	1581.26	Joback Method
cpg	2367.39	J/mol×K	1650.72	Joback Method
cpg	2461.48	J/mol×K	1720.18	Joback Method
cpg	2568.53	J/mol×K	1789.64	Joback Method
cpg	2690.14	J/mol×K	1859.10	Joback Method
cpg	2827.90	J/mol×K	1928.56	Joback Method

Sources

Thermodynamic Properties of Polymorphs of 2,2'-Thiodiethylene Bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]: https://www.doi.org/10.1021/je500869p

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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